The Impact of Biomass Fuels on Flame Structure and Pollutant Formation during Biomass Cofiring Combustion

Melissa Lauren Holtmeyer
Washington University in St. Louis

Follow this and additional works at: https://openscholarship.wustl.edu/etd

Recommended Citation
https://openscholarship.wustl.edu/etd/1007

This Dissertation is brought to you for free and open access by Washington University Open Scholarship. It has been accepted for inclusion in All Theses and Dissertations (ETDs) by an authorized administrator of Washington University Open Scholarship. For more information, please contact digital@wumail.wustl.edu.
The Impact of Biomass Fuels on Flame Structure and Pollutant Formation during Biomass Cofiring Combustion

by

Melissa Lauren Holtmeyer

A dissertation presented to the Graduate School of Arts and Sciences of Washington University in partial fulfillment of the requirements for the degree of Doctor of Philosophy

December 2012

St. Louis, Missouri
Table of Contents

List of Figures ........................................................................................................................................... v
List of Tables ............................................................................................................................................... viii
Acknowledgements ..................................................................................................................................... ix
Dedication ................................................................................................................................................... x
Abstract ....................................................................................................................................................... xi

1 Introduction .............................................................................................................................................. 1
  1.1 Background ........................................................................................................................................ 1
  1.2 NO Formation ................................................................................................................................... 6
    1.2.1 Fuel NOx .................................................................................................................................... 6
    1.2.2 Thermal NOx .......................................................................................................................... 7
    1.2.3 Prompt NOx .............................................................................................................................. 7
    1.2.4 Approaches for NOx reduction ................................................................................................. 7
  1.3 LACER previous work: Oxyfuel combustion for NOx reduction ..................................................... 9

2 Research Objectives ............................................................................................................................... 12

3 Experimental methods ............................................................................................................................ 16
  3.1 Laboratory-scale combustion furnace ........................................................................................... 16
  3.2 In-flame gaseous species and particle sampling ............................................................................. 18
    3.2.1 Flame length measurements .................................................................................................... 19
  3.3 Fuels .................................................................................................................................................. 20
  3.4 Chapter Summary ............................................................................................................................. 21

4 Numerical methods .................................................................................................................................. 22
  4.1 Introduction ....................................................................................................................................... 22
  4.2 Summary of model specifications ................................................................................................. 25
  4.3 Grid Construction ............................................................................................................................ 27
    4.3.1 Grid refinement study ............................................................................................................. 28
  4.4 CFD Methods ................................................................................................................................... 32
    4.4.1 Convergence Criteria ............................................................................................................. 33
    4.4.2 Boundary conditions .............................................................................................................. 33
    4.4.3 Turbulence and turbulent interactions .................................................................................... 35
      4.4.3.1 Turbulence-chemistry interactions ................................................................................. 37
      4.4.3.2 Turbulence-radiation interactions ................................................................................... 39
    4.4.4 Discrete phase model .............................................................................................................. 40
      4.4.4.1 Coal devolatilization law ................................................................................................. 42
      4.4.4.2 Coal char combustion model .......................................................................................... 46
      4.4.4.3 Biomass devolatilization model ....................................................................................... 46
      4.4.4.4 Biomass char combustion model ...................................................................................... 48
    4.4.5 Radiation model ...................................................................................................................... 48
    4.4.6 NOx model ............................................................................................................................. 50
5 The impact of biomass fuels on volatile flame length .................................................. 56
  5.1 Introduction ............................................................................................................... 56
  5.2 Volatile flame length of a coal flame ......................................................................... 57
  5.3 Volatile flame length during biomass cofiring .......................................................... 60
  5.4 Impact of particle breakthrough on volatile flame length .......................................... 62
  5.5 Biomass particle size .................................................................................................. 63
  5.6 Cofiring ratio ............................................................................................................. 65
  5.7 Systematic study of biomass particle size for breakthrough in air-fired and oxyfuel
      combustion conditions ............................................................................................... 69
      5.7.1 Air-fired flames ................................................................................................. 70
      5.7.2 Oxy-cofired flames ........................................................................................... 73
  5.8 Chapter Summary ...................................................................................................... 75

6 Relationship between volatile flame length and NO formation ............................. 76
  6.1 Introduction ............................................................................................................... 76
  6.2 Cofiring ratio impacts on NO formation .................................................................... 78
      6.2.1 Air-fired conditions ......................................................................................... 78
      6.2.2 Oxyfuel conditions ......................................................................................... 79
  6.3 Other considerations for increased NO emissions .................................................... 80
  6.4 Chapter Summary ...................................................................................................... 81

7 Criteria for particle breakthrough of the volatile flame ........................................ 82
  7.1 Introduction ............................................................................................................... 82
  7.2 Basic approach ......................................................................................................... 83
  7.3 Structure and processes of volatile flame formation in solid fuel combustion .......... 84
      7.3.1 Nonpremixed turbulent gaseous flame ............................................................ 85
      7.3.2 Turbulent mixing ............................................................................................ 86
      7.3.3 Particle devolatilization process ..................................................................... 88
  7.4 Flame and particle devolatilization time scales ...................................................... 89
      7.4.1 Prediction of nonpremixed turbulent flame length ........................................ 89
      7.4.2 Group combustion for solid fuel burning ....................................................... 91
      7.4.3 Single particle devolatilization ...................................................................... 92
  7.5 Dimensionless number for particle breakthrough prediction .................................. 94
  7.6 Chapter Summary ...................................................................................................... 97

8 Conclusions and recommendations ........................................................................... 98
  8.1 Conclusions ............................................................................................................... 98
  8.2 Recommendations for future work .......................................................................... 100

Appendix A: Supplementary CFD material .................................................................. 102
  A.1 CFD methods .......................................................................................................... 102
  A.2 Conservation equations ............................................................................................ 103
  A.3 Conversation equations for swirling flow .............................................................. 104
  A.4 Spatial discretization ............................................................................................... 105
  A.5 Segregated solver algorithm .................................................................................... 107
List of Figures

Figure 1.1. NO emissions vs. mass percentage of wood waste (<18 mesh) cofired with coal at a thermal input of 30 kW [25] .................................................................10

Figure 1.2. NO emissions versus the mass percentage of reduced size wood waste (<50 mesh) cofired with coal for 30 kW flames [25] .................................................................10

Figure 3.1. Experimental pulverized fuel combustion system ........................................16
Figure 3.2. Experimental profiles of CO fraction along the centerline of 18 kW coal, 20 wt.% cofired, and 40 wt.% cofired flames .................................................................20

Figure 4.1. Near burner region (burner and start of combustion chamber) geometry and discretization a) 2D and b) 3D configurations .................................................................28

Figure 4.2. Axial velocity profiles for two-dimensional coal flame calculations with varying cell sizes located at a) port 3 (0.23m away from the burner outlet), b) port 7 (0.91m away from burner outlet), and c) port 9 (1.45m away from burner outlet) ..................................30

Figure 4.3. Centerline volatile release profiles for two-dimensional coal flame calculations with varying cell sizes .................................................................31

Figure 4.4. Axial temperature profiles for two-dimensional coal flame calculations with varying cell sizes located at a) port 3 (0.23m away from the burner outlet), b) port 7 (0.91m away from burner outlet), and c) port 9 (1.45m away from burner outlet) ..................................32

Figure 4.5. Axial velocity profiles of flow field solutions at port 3 (22.9cm away from the burner outlet) and varying SO\textsubscript{2} inlet definitions with and without tangential velocity decay ........35

Figure 4.6. Centerline CO fraction profiles for two-dimensional coal flame solutions with varying turbulent closure models .................................................................37

Figure 4.7. Centerline CO fraction profiles for two-dimensional coal flame solutions with varying turbulent-chemistry interaction models .................................................................39

Figure 4.8. Particle tracks for a) coal particles and b) biomass particles in a 20 wt.% cofired flame in the laboratory-scale system .................................................................41

Figure 4.9. Centerline CO fraction profiles for two-dimensional coal simulations with varying devolatilization models .................................................................44

Figure 4.10. Centerline CO fraction profiles for two-dimensional coal simulations with varying global kinetic reaction mechanisms .................................................................45

Figure 4.11. Centerline CO fraction experimental measurements in propane flames with varying sampling locations in the combustion chamber and fuel feed rate .........................................52

Figure 4.12. Temperature contours for a) two-dimensional and b) three-dimensional propane flame simulations with the end of the flame located at port 5 .................................................................53
Figure 4.13. a) Numerical contours of stream function and b) numerical velocity vectors colored by axial velocity for two-dimensional propane flame simulations .................................................. 54

Figure 5.1. Description of the structure of pulverized fuel flames (picture is a pulverized coal and gas flame courtesy of the LACER lab) ........................................................................................................ 56

Figure 5.2. Centerline CO fraction experimental measurements in coal flames with varying sampling locations in the combustion chamber and fuel feed rates ........................................ 58

Figure 5.3. a) Experimental and numerical profiles of CO fraction (−) and numerical volatile reaction rate with oxygen (---) along the centerline and of an 18 kW coal-fired flame. b) Numerical contours of temperature for the same flame ...................................................... 59

Figure 5.4. Experimental and numerical profiles of CO fraction (−) and total volatile reaction with oxygen (---) for a 18 kW 20 wt.% cofired flame with wood waste (< 18 mesh). The arrow denotes the end of the volatile flame ................................................................. 61

Figure 5.5. Pulverized fuel flame schematics for a) no particle breakthrough of the volatile flame and b) particle breakthrough of the volatile flame. The gray areas represent the char burnout zone ...................................................................................................................... 62

Figure 5.6. Experimental and numerical profiles of CO fraction (−) and volatile reaction with oxygen (---) for an 18 kW 20 wt.% cofired flame with the reduced particle size wood waste (< 40 mesh). The arrow denotes the end of the volatile flame ................................................................. 64

Figure 5.7. Numerical profiles of particle breakthrough of the volatile flame and volatile flame length of cofiring with the original wood waste (< 18 mesh) ................................................................. 65

Figure 5.8. Experimental and numerical profiles of CO fraction (−) and volatile reaction with oxygen (---) for a 18 kW 40 wt.% cofired flame with wood waste (< 18 mesh). The arrow denotes the end of the volatile flame ................................................................. 66

Figure 5.9. Numerical profiles of particle breakthrough of the volatile flame and volatile flame length of cofiring with small (<40 mesh) wood waste .............................................................................. 67

Figure 5.10. Numerical profiles of particle breakthrough of the volatile flame and volatile flame length of cofiring with industrial-size biomass .............................................................................. 68

Figure 5.11. Numerical profiles of CO fraction (−) and volatile reaction with oxygen (---) along the centerline of an 18 kW 20 wt.% cofired flame with industrial size wood waste. The arrow denotes the end of the volatile flame .............................................................................. 68

Figure 5.12. a) Numerical temperature contours and b) volatile reaction rate with oxygen for 30 kW coal flame. Arrows denote the volatile flame length .............................................................................. 70

Figure 5.13. Numerical contours of temperature contours for 20 wt.% cofired flames with wood particle sizes of a) the same size distribution as coal, b) 600 μm monodisperse size distribution c) 1 mm monodisperse size distribution .............................................................................. 71

Figure 5.14. Numerical centerline temperatures for 20 wt.% cofired flames with wood waste of varying particle sizes: the same particle size distribution as coal (−), 600 μm monodisperse (−−−), and 1 mm monodisperse (−−−−) .............................................................................. 72

Figure 5.15. a) Centerline temperatures for a coal flame (−) and a 20 wt.% cofired flame (−−−) using a b) theoretical particle size distribution of wood to truncate peak temperatures ......... 73

Figure 5.16. Temperature contours for 20 wt.% cofired flames with 600 μm wood particles during a) air-fired and b) oxyfuel combustion conditions .............................................................................. 74
Figure 6.1. Contours of NO mole fraction for 30 kW a) coal flame and 20% cofired flames with wood particle sizes of b) the same size distribution as coal, c) 600 μm monodisperse size distribution d) 1 mm monodisperse size distribution.

Figure 7.1. Schematic of flame and particle processes occurring in the near burner zone at levels of a) nonpremixed turbulent gaseous flame, b) eddy mixing and entrainment of gases and particles, c) group combustion of particles within eddies, and d) single particle devolatilization leading to the release of volatile gases from the particle.

Figure 7.2. Numerically predicted critical size of biomass particles to breakthrough the volatile flame before complete devolatilization for $VF# = 1$ of 18 kW cofired flames with varying % biomass.
List of Tables

Table 3.1. Ultimate & proximate analyses ................................................................. 21
Table 3.2. Sieve analysis ......................................................................................... 21

Table 4.1. Model Specifications for CFD simulations .................................................. 26
Table 4.2. Computational mesh specifications .......................................................... 29
Table 4.3. Kinetic data for volatile reaction mechanism ............................................. 45
Table 4.4. Kinetic data for char surface reactions ..................................................... 46
Table 4.5. Propane flow rates at the end of the flame ............................................... 53

Table 5.1. Volatiles remaining in particles sampled along the centerline ................. 65
Table 5.2. Inlet flow rates for 30 kW air-fired and oxyfuel combustion ...................... 75

Table 6.1. Summary of NO emissions from 30 kW air-fired conditions .................... 80
Table 6.2. Summary of NO emissions from 30 kW oxyfuel conditions ...................... 82
Acknowledgements

This work was funded by the National Aeronautics and Space Administration (NASA) under the Missouri Space Grant Consortium, the Consortium for Clean Coal Utilization at Washington University in St. Louis, and the United States Environmental Protection Agency (U.S. EPA) under the Science to Achieve Results (STAR) Graduate Fellowship program.

This Ph.D. dissertation was developed under STAR Fellowship Assistance Agreement no. FP-91715901-2 awarded by the U.S. Environmental Protection Agency (EPA). It has not been formally reviewed by EPA. The views expressed in this Ph.D. dissertation are solely those of Melissa Holtmeyer and her colleagues, and EPA does not endorse any products or commercial services mentioned in this Ph.D. dissertation.

It has been an honor to work with my advisor, Dr. Richard L. Axelbaum. Deep gratitude is expressed for his guidance, curiosity, and ability to enable me to perform this work as well as pursue opportunities outside of the lab. It was his encouragement and support that has helped me become a successful research scientist and an accomplished graduate student leader at WU. He embraced my creativity, while pushing me to gain a deeper understanding of subject of this dissertation. For this I am forever grateful.

I would also like to thank the members of my dissertation committee Professors Pratim Biswas, Jay R. Turner, Palghat A. Ramachandran, Milorad P. Dudukovic, Ramesh K. Agarwal, and Steven H. Frankel for their support and guidance. The technical assistance and support of my colleagues, specifically Yosef Santer and George Pires, in the Laboratory for Advanced Combustion and Energy Research is also acknowledged.

Special thanks are given to Dr. Benjamin M. Kumfer and Dr. Scott Skeen. Dr. Kumfer provided me with tremendous assistance and feedback throughout this work as well as his ability to always keep me focused on the task at hand. His outlook on the future of this field as well as his ability to see the bigger picture are inspiring. Dr. Skeen completed the NO emissions work, which provided the direction for this dissertation. He drove me to dig deeper and become a more focused researcher.

Melissa L. Holtmeyer

Washington University in St. Louis
December 2012
Dedicated to my friends...

Who have been the best friends a girl could ask for. I am forever grateful for their unwavering support in my graduate work as well as my other endeavors. Their abilities to keep me laughing and enjoying life has enabled me to accomplish more than I would have ever imagined. Thank you for everything: Greg, Warren, Theresa, Kat, Steve, Katie E., Tess, Katie T., Mary, Dan, Mehmet, and Evgeniy.

Dedicated to my family...

Without you, none of this would have been possible. You have kept me grounded and provided me with so much throughout my life. To my Mom and Dad: I am forever grateful to you for all that you have done to enable me to pursue my dreams. To Brandi: You are my inspiration. To Gus: Your love and encouragement motivate me to be the best that I can be in life and in my career.
Cofiring of biomass in pulverized coal boilers for large-scale power generation requires that current combustion standards of stability, reliability, emission and fuel conversion efficiency are maintained and/or improved. While the properties of biomass fuels are highly variable and can differ significantly from that of coal, in general biomass fuels have greater volatile matter content and larger particle size. The larger size is due to both fuel preparation methods as well as the physical properties of the biomass material. These two characteristics significantly impact the structure of the volatile flame, which is the zone dominated by the combustion of volatiles in the near burner region. The length and location of the volatile flame is important not only to flame stability, but also to the formation of pollutants such as NOx. Previous experiments have shown an increase in N conversion to NO when cofiring during both air-fired and oxyfuel combustion, despite the wood waste having less fuel-bound nitrogen. CFD simulations reveal that the impact of biomass fuels on the volatile flame length lead to increased NO formation.
Changes in volatile flame structure and NO formation are investigated using experimental and computational fluid dynamic (CFD) methods for cofired flames of pulverized coal and wood waste. Volatile flame length is measured experimentally using gaseous species measurements of CO and CO$_2$ in a 35 kWth combustion facility. A numerical study aids in the interpretation of the impacts of wood waste on the volatile flame. Lastly, a simple model is developed to predict the effects of particle size on flame length. A dimensionless number, the Volatile Flame Number ($VF#$), assists in the comparison of flame and particle devolatilization processes.

The length of the fuel-rich volatile flame zone is found to be sensitive to the location of volatile matter release and the amount of volatiles available in the near burner region. Larger particles with high axial momentum and longer heating times breakthrough the volatile flame zone to release volatiles downstream into areas rich in oxygen. The delayed release of volatiles leads to less volatiles in the fuel-rich region and shorter volatile flames, which augments breakthrough of particles before complete release of volatiles. Increased volatile matter content, characteristic of biomass fuels, leads to an increased volatile flame length and reduced particle breakthrough when all volatiles are released in the near burner region. Particle breakthrough is shown to occur for all biomass cofired flames, but the critical size for breakthrough occurs for low cofiring ratios due to the significant particle size difference between coal and wood waste. As the cofiring ratio increases, so does the participation of wood particles in the volatile flame leading to longer flames and less breakthrough. This work will demonstrate that flame structure can be optimized for desired volatile flame lengths and minimum emissions by selecting biomass properties such as particle size and volatile matter content.
1 Introduction

1.1 Background

The combustion of pulverized coal provides 42% of the electricity generated in the U.S. and, similarly, 43% of the electricity generated worldwide [1]. Centralized coal-fired power infrastructure is composed of large power plants that are interconnected via the transmission and distribution system to provide electricity at all times across the nation. Electricity generation from pulverized fuel power plants is a successive conversion process from chemical energy, thermal energy, mechanical energy and, lastly to electrical energy. Chemical energy in the form of heat and gases from solid fuel combustion is converted into thermal energy in the form of steam, which is used to run turbines that ultimately power the electric generator. Heat transfer (convection and radiation) from turbulent pulverized fuel flames is utilized to heat water in boiler tubes that line the walls of the furnace. In a 500 MW power plant, for example, 24 burners (i.e. 24 flames) generate the necessary heat to run the steam turbines [2]. Pulverized fuel flames have been optimized for large-scale power generation to minimize pollutant emissions and attain maximum fuel conversion. This traditional way of producing power is facing new challenges due to rising CO₂ emissions, criteria pollutant emission regulations, and renewable portfolio standards (RPS). The impact of new combustion technologies to address these challenges is significant due to the large number pulverized fuel power plants around the world.

New approaches to pulverized fuel combustion are needed to address today’s challenges as well as meet increasing electricity demands. Over the past 50 years, the ultimate goal of coal-fired power to provide reliable electricity has remained, but the constraints, especially on emissions,
have evolved. In the 1960’s, the power generation industry was beginning with the primary objective of getting capacity and electricity to the consumers [3]. In the 1970’s, while the industry was still expanding, the U.S. Environmental Protection Agency (U.S. EPA) passed the Clean Air Act of 1970 bringing about federal government involvement in air pollution control [4]. The objectives were to, not only continue to build capacity, but to also limit emissions. From the 1980’s until today, the objectives have been to maintain the power plants previously constructed and to continue to reduce emissions. Throughout this history, combustion processes and, consequently, flame structures have evolved to meet new regulations and power plant operations.

While the use of coal has been instrumental to the world’s advancement, some by-products of the combustion process can have adverse effects on the environment and human health if released. Sulfur oxides (SOx), nitrogen dioxide (NO₂), and particulate matter (PM) are criteria pollutants used by the U.S. EPA as indicators for air quality. SOx and NOx are gaseous species formed in the flame and found in parts-per-million (PPM) level concentrations, which can be reduced or eliminated by combustion modifications and/or flue gas treatment. Particulate matter, such as soot and fly ash, can be also be captured using flue gas treatment. NOx has been linked to acid rain and smog formation, while long term exposure to high levels of NOx and SOx have been associated with cardiovascular and respiratory illnesses [5]. Exposure to PM can also have detrimental human health effects, specifically cardiovascular impacts [5,6].

Carbon dioxide is major product of combustion and is also a greenhouse gas (GHG), which can trap heat in the atmosphere. Anthropogenic greenhouse gas emissions, especially CO₂, are increasingly impacting the climate. The natural CO₂ cycle involves both addition and removal from the atmosphere, but emissions from human activities are adding more CO₂ than is being removed. Carbon dioxide is a radiatively active gas and a major contributor to radiative forcing,
which impacts the trapping of heat within the earth’s atmosphere [7]. Of the CO₂ emitted by the U.S., 40% comes from electricity generating sources [1]. Unlike treatments for other pollutants, CO₂ cannot be eliminated with combustion modifications, and is expensive to capture and store, which would reduce or eliminate CO₂ emissions. If pulverized fuel combustion is to continue, CO₂ reduction and/or elimination coupled with further reductions of all other pollutants needs to be a major consideration for future technologies.

Today’s decisions around power generation are no longer just about technology and finances, but also consider social, political, and environmental factors. Renewable energy technologies, including biofuels, solar and wind power, and new coal related technologies, including integrated gasification combined cycle (IGCC), biomass cofiring, and oxy-coal combustion, have entered the large-scale power generation sector, namely because of the consideration of non-technical issues. Multicriteria considerations for decision-making provide a well-rounded approach for to determine appropriate technologies. Scale, location, reliability, centralized vs. distributed generation, costs, electricity demand, and environmental impacts are among the important variables that should be addressed for the selection of power generation sources [8]. Further discussions and application of this approach are included a paper titled “Considerations for decision-making on distributed power generation in rural areas” (Appendix C). In making near-term decisions towards carbon-free power generation, power plants should implement advanced technologies while utilizing the current infrastructure.

Biomass cofiring is a technology that maintains the traditional method of power generation, while reducing emissions and potentially meeting RPS. The utilization of biomass fuels to supplement large-scale coal-fired power has opportunities and challenges in areas of combustion, logistics, and infrastructure. The composition of biomass fuels can be widely variable and differ significantly from those of coal, which impacts both combustion and logistics
of biomass use. While logistics and infrastructure are important issues for large-scale deployment, this work only focuses on combustion. Ultimate and proximate analyses generally vary from one biomass to another, but can also vary within a single fuel type. Biomass fuels can vary significantly from each other in elemental composition and physical appearance and can have several different botanic fractions with wide variations in chemical compositions [9,10]. Fahmi et al. [10], found that botanic fractions within energy grasses vary in lignocellulosic composition and metal contents. Energy grasses typically have four botanic fractions, while corn stover species have at least six, including nodes, piths, rinds, sheaths, husks and leaves [11].

Biomass-fired power has been used worldwide to meet local and large-scale demands. The European Union has been a leader in research efforts and large-scale utilization of biomass for power generation, namely due to CO₂ legislation to reduce emissions [12]. The large sugarcane industry in Brazil provides millions of tons of bagasse, annually, to power on-site mills and has plans for future expansion of bagasse use for large-scale power generation [13]. The U.S., on the other hand, has small demonstrations, but does not have the regulatory or political framework to regulate carbon emissions and/or to promote the use of biomass [14–18]. Utilization of biomass in the large-scale power generation sector could reduce the overall CO₂ emissions of the U.S. utilities sector by 100 million tons per year by displacing fossil fuel combustion with the near carbon-neutral combustion of biomass [19]. With uncertainties about carbon regulation and the future of U.S. energy policy, power generation utilities are unsure about making large changes to include biomass. However, with the rising energy demands and the direction that other countries have taken in response to carbon regulations, biomass cofiring should be considered as a key technology in the energy portfolio.

Oxyfuel combustion with carbon capture and storage (CCS) and biomass cofiring, individually and in combination, are both approaches to coal-fired power that can contribute to the
reduction of CO$_2$ emissions. Oxyfuel combustion enables CCS by burning fuels with a combination of oxygen and recycled flue gas instead of air. The flue gas is primarily composed of CO$_2$ and H$_2$O. The water is condensed out to create a concentrated CO$_2$ stream for geological storage. Oxyfuel combustion combined with geological storage is a near-zero emission technology that can be applied to both existing and new coal-fired power plants [20–22]. By combining oxyfuel combustion and biomass cofiring with CCS, oxy-cofiring combustion can be a potentially carbon negative generation technology. Accordingly, this approach has been identified as a technology that can be utilized to stabilize atmospheric CO$_2$ emissions [23]. Other potential benefits include utilization of waste or difficult to burn fuels that would have otherwise been unusable in air-fired conditions. At this time, little is known about the impacts of oxy-cofiring on combustion performance and pollutant formation.

Combustion is the oldest technology of humankind and has been a major energy source for over one million years [24]. However, to meet future electricity demands and needs for cleaner power, the approach to large-scale combustion needs to be reinvented. Historically, pulverized fuel flame research has focused on power plant design and the understanding of basic processes for fuel decomposition and chemical heat release. The approaches used today should build on this basic knowledge, and also aim to advance pulverized fuel combustion for its continued use. New combustion environments and fuels can create unexpected problems and/or benefits that need to be better understood. This work will investigate flame structure and NOx formation in biomass cofired flames during air-fired and oxyfuel combustion with an emphasis on understanding changes in the combustion process.

Studies completed prior to this work in our research group laid the foundation for focusing on how changes in flame structure can impact NO emissions in biomass cofired flames. While NO emissions have been well characterized in traditional systems, the important findings from
Skeen et al. [25,26], which are summarized in the following sections, provide evidence of the complicated nature of NOx formation when utilizing advanced combustion techniques.

1.2 NO formation

Nitrogen oxides, such as nitric oxide (NO), nitrogen dioxide (NO\(_2\)), and nitrous oxide (N\(_2\)O) are all products of the combustion process. Nitrogen oxide species can be formed from the oxidation of molecular N\(_2\) in the combustion air and the oxidation of nitrogen released from the solid fuel. A large body of literature exists on the combustion modifications and/or post-combustion treatment processes that can reduce or even eliminate NOx emissions. The following sections include an overview of the NOx formation mechanisms that occur during pulverized fuel combustion.

1.2.1 Fuel NOx

Fuel-bound nitrogen is partitioned between volatile-N, which releases with the gaseous volatiles during devolatilization and char-N, which remains on the char surface. Fuel-N reacts to form nitrogen-containing intermediates, such as hydrogen cyanide (HCN) or ammonia (NH\(_3\)) [27]. Depending on the local combustion conditions including temperature, species, and residence time, HCN and NH\(_3\) react with oxygen to form NO or react with other nitrogen-containing intermediates to reduce to N\(_2\) [28]. The oxidation of fuel-N is the main source of NO contributing to over 75% of the total NO emissions with volatile-N conversion to NO dominating over char-N conversion [29].
1.2.2 Thermal NOx

Thermal-NO is formed from \( \text{N}_2 \) that enters with the combustion air. At high temperatures, breaking of the nitrogen triple bond is favored leading to the availability of nitrogen-containing intermediates [30]. The Zel'dovich mechanism, which describes the formation of thermal-NO as shown in Equations 1.1, 1.2, and 1.3, does not produce significant concentrations of NO until temperatures exceed 1800 K. The potential contribution of thermal-NO in air-fired conditions can be significant at high temperatures, but with low NOx burner technologies the contribution is much lower [31].

\[
\text{N}_2 + \text{O} \rightarrow \text{NO} + \text{N} \quad (1.1)
\]
\[
\text{O}_2 + \text{N} \rightarrow \text{NO} + \text{O} \quad (1.2)
\]
\[
\text{N} + \text{OH} \rightarrow \text{NO} + \text{H} \quad (1.3)
\]

1.2.3 Prompt NOx

The attack of the \( \text{N}_2 \) triple bond with fuel-derived radicals such as C, \( \text{CH} \), or \( \text{CH}_2 \) results in the formation of nitrogen-containing intermediates such as nitrogen monohydride (NH), HCN, or cyano radicals (CN-), which can oxidize to form NO [28,30]. For pulverized fuel combustion, the contribution from the prompt NOx mechanism is typically very small (~5%) [32]. Approaches that are used to reduce fuel and thermal NOx, also work to reduce prompt NOx.

1.2.4 Approaches to NOx reduction

Conventional approaches to combustion modification for NOx reduction include both in-flame methods, which are applied at the individual burners, and in-furnace methods, which modify the combustion environment of the boiler. Key in-flame strategies to reduce thermal-NO reduce the near burner combustion temperatures to eliminate the potential for \( \text{N}_2 \) dissociation. Key
strategies to reduce fuel-NO include oxidizer or air-staging, which can be adopted at the in-flame or in-furnace level, create a reducing environment for NO conversion to $N_2$. For industrial boilers, operating with many burners, the upstream burners will supply insufficient oxidizer, while downstream, the remaining air to complete combustion is supplied. This can also be accomplished in individual burners through quarl-based designs creating a fuel-rich near burner zone [33–35].

Similar to the concept behind oxidizer-staging, fuel-staging (or reburning) involves injecting fuel downstream creating a fuel-rich zone reducing NOx species to $N_2$ [36,37]. Lastly, NOx emissions can also be reduced by post-combustion gas treatment methods including selective non-catalytic reduction (SNCR) or selective catalytic reduction (SCR).

Besides burner modifications and post-combustion gas cleanup methods, oxidizer gas composition and fuel selection can be modified to further reduce NOx emissions. In oxyfuel combustion, $N_2$ from the combustion air is eliminated by burning fuels in pure oxygen and recycled flue gas (RFG), which is primarily composed of $CO_2$. Nitrogen oxide emissions can be reduced by as much as 70% compared to air-fired conditions [20,38–43], primarily through the elimination of the thermal-NO mechanism. Other reductions have been reported from char and recycled NOx reactions [39,44,45].

Cofiring with biomass can also potentially reduce NOx emissions. With the variability of biomass fuel chemical compositions, fuel-N contents also vary. However, cofiring biomass fuels with lower fuel-N than coal does not always guarantee lower NO emissions. NOx formation is highly complex and dependent upon many factors throughout the combustion process. The experimental work in the following sections focus on the changes in NO emissions during biomass cofiring in air-fired and oxyfuel combustion conditions.
1.3 LACER previous work: Oxy-fuel combustion for NOx reduction

Skeen et al. [25,26] experimentally investigated the effects of varying cofiring ratio on NO emissions during air-fired and oxyfuel combustion. In all experiments, conditions were set such that the thermal input was maintained at 20 kW and 30 kW with the exhaust gas oxygen concentrations maintained at 3 vol.% O₂. Under oxyfuel conditions, flue gases were not recycled; rather, a once-through system with a ratio of 30 vol.% O₂/70 vol.% CO₂ was used to determine the effects of N₂ replacement with CO₂, while maintaining similar adiabatic flame temperatures and heat flux to that of air-fired conditions [46].

From this work, N conversion to NO increased with cofiring ratio, resulting in higher than expected NO emissions based on fuel nitrogen content, during both air-fired and oxyfuel combustion as is shown in Figures 1.1 and 1.2. The air-fired 20 kW case became unstable as the cofiring ratio increased. Unstable flames entrained oxygen at the base of the flame resulting in increased oxygen concentrations in the near burner region and increased NO. For the 30 kW 40 wt.% cofired flames, N conversion to NO increased 14% and 32% for air-fired and oxyfuel combustion, respectively, compared to the coal only flame. The wood waste has less fuel-N (see Table 3.1), which would lead one to expect a decrease in NO emissions. However, when the wood particle size was reduced by sieving with a 50 mesh sieve, a reduction in NO emissions was observed under air-fired conditions. With the reduced wood particle size, NO emissions decreased by 15% for 40 wt.% cofiring (Figure 1.2) compared to 40 wt.% cofiring with the larger wood waste (Figure 1.1).
During oxyfuel conditions, NO emissions were reduced over the air-fired case, largely due to the elimination of the thermal-NO mechanism. However, unlike the air-fired case, NO emissions remained constant even when cofiring the reduced particle size wood waste. With gaseous inlet conditions held constant for the coal and cofired cases, these results suggest that the addition of wood waste is impacting the flame structure leading to increased NO formation. Therefore, knowledge of the near burner zone conditions and the volatile flame are important for understanding the potential for NO emission reductions when cofiring with biomass fuels.
2 Research Objectives

The addition of biomass to coal flames in large-scale coal-fired power plants has the potential to alter the combustion process. The properties of biomass fuels can vary significantly from those of coal leading to complex interactions, which if gone unnoticed, can negatively impact the combustion process and formation of pollutants. This work aims to identify flame and particle interactions that control flame structure, while determining the potential impacts of changes on pollutant formation, specifically NOx. The impacts of biomass fuels on the volatile flame zone during biomass cofiring will be observed during air-fired and oxyfuel combustion conditions.

Possible flame length and emission changes are identified utilizing laboratory-scale experiments, CFD, and scaling methods. While laboratory-scale systems are easier to operate and more detailed measurements can be obtained than in industrial-scale systems, there are still limitations. The 35 kWth laboratory-scale furnace used in this work has realistic flame characteristics leading to harsh environments and the need for durable furnace construction to reduce heat losses. Detailed in-flame measurements of pulverized fuel flames are difficult due to the harsh environment and the limited access to get sampling probes into the flame. However, measurements at discrete locations throughout the combustion chamber can provide information about the basic features of flame behaviors. Due to the limited experimental capabilities, CFD simulations can provide insight, identify new phenomena, and determine the controlling features of pulverized fuel flames. Important experimental measurements that can provide basic information about potential changes are emissions, which are taken at the exhaust of the combustion chamber.
The experimental NO emission findings in Section 1.3 provide a basis to understand the flame processes in more detail. The primary source of NO emissions in both air-fired and oxyfuel combustion conditions is fuel-NO (Section 1.2.1), which can form from volatile-N or char-N. This work focuses on the structure of the volatile flame region and how particles interact with this zone. The volatile flame zone is the region dominated by the combustion of gaseous volatiles and has an intense emissive power enhanced by soot formation [47,48]. The addition of biomass particles and/or new combustion gas compositions directly impacts the volatile flame, and ultimately fuel-N conversion to NO.

The goal of this work is understand the combustion conditions and biomass fuel characteristics that can lead to increased NO emissions as well as changes in volatile flame structure during biomass cofiring using experimental, numerical, and scaling methods. These changes in structure can also have implications for other formation processes (i.e. loss-on-ignition and particulate matter), which are not studied here.

The length of pulverized fuel flames has been studied in the past, but has included the end of char burnout [49–52], with the volatile flame included in that length. Total length of pulverized fuel flames, including the char burnout zone, is important for combustion chamber and boiler design. However, power plants currently operating are in need of new combustion approaches to meet emission regulations, while still achieving maximum fuel conversion, which implies that a more detailed understanding of the volatile flame structure and particle interactions is needed. Detailed studies on volatile flame length in pulverized fuel flames, especially biomass cofiring and oxyfuel combustion flames, have not been completed to the author's knowledge. The approach developed in this work to study volatile flame structure of pulverized fuel flames includes the following methods:
1. Develop in-flame measurement techniques to experimentally determine the volatile flame length and to validate the CFD code. Species measurements of CO and CO$_2$ at discrete locations along the centerline length of the combustion chamber will be used to determine the end of the volatile flame.

2. Determine the impacts of biomass fuels on the volatile flame length by varying biomass particle size, overall volatile fraction, and cofiring ratio. Experimental measurements provide evidence of changes in volatile flame length, while CFD simulations offer detailed information on the causes and the presence of particle breakthrough of the volatile flame before complete devolatilization.

3. Understand the conditions of particle breakthrough with a systematic numerical study of biomass particle size using monodisperse size distributions for air-fired and oxyfuel combustion conditions. The impacts of particle breakthrough on NO formation and emissions will be compared as well as validated against the trends from previous experimental data presented in Section 1.3.

4. Develop a simple model using scaling methods to predict the presence of particle breakthrough of the volatile flame before complete devolatilization. Time and length scales of flame and particle devolatilization processes can be calculated and compared to determine to the overall participation of volatiles in the volatile flame length.

The remaining chapters will focus on the methods used to complete this work and the important findings. Chapter 3 provides descriptions of the laboratory-scale experimental system, fuels, and measurement techniques using species concentrations. Examples of experimental data completed in this work are also presented. While, Chapter 4 discusses the details of the CFD
model and the specific solid fuel combustion sub-models that were chosen to capture the behaviors of the volatile flame length and particle breakthrough. Model sensitivities, grid independence, and validation experiments are also introduced. The structure of pulverized fuel flames, specifically the volatile flame, is described in Chapter 5. Changes in volatile flame length with respect to the overall volatile fraction of the fuels and biomass particle size are analyzed using both experimental and CFD methods. The complex relationship between particle breakthrough of the volatile flame before complete devolatilization and volatile flame length with be discussed. The implications of particle breakthrough on NO formation are discussed in Chapter 6 for air-fired and oxyfuel conditions. Lastly, Chapter 7 describes the development of simple model to predict the presence of particle breakthrough based on scaling methods of flame and particle devolatilization processes as well as important factors and actions that can be taken to prevent particle breakthrough. A new dimensionless number that was developed to characterize conditions of particle breakthrough will also be discussed.
3 Experimental Methods

3.1 Laboratory-scale combustion furnace

Experiments were conducted in a cylindrical, horizontally-fired 35 kWth combustor designed with a 16.7 cm ID combustion section, 2.43 m in length, followed by a 37 cm ID burnout section, 120 cm in length (Figure 3.1). The secondary oxidizer (SO) flow was introduced with axial and tangential components, creating a swirling flow to assist in flame stabilization. Pulverized coal and wood waste were fed to the combustor using separate volumetric screw feeders (K-Tron and Schenck AccuRate, respectively) and were entrained into the primary oxidizer (PO) stream using an eductor. The two feeder outlets and the eductor were contained within an enclosure maintained at atmospheric pressure, and the gases flowing into the fuel inlet of the eductor were controlled and measured. No buoyancy-induced asymmetries in the flow field were observed.

Several combustion chamber modifications were completed to have better access to the near burner flame region and to improve the overall robustness of the system. The combustion section was doubled in length as well as reconstructed with a 6.4 cm thick ceramic refractory lining and sampling ports along the length. The particulate matter filter was also added during this work.
Gas flows and compositions of the PO and SO were controlled independently using calibrated rotameters. The combustion chamber and the educator/feeder outlets were sealed to prevent air infiltration. The exhaust outlet of the combustion chamber was connected in line with a particulate matter filter, which was followed by the building exhaust. The pressure drop across the filter was maintained around 6 inH₂O of a slight positive pressure upstream (ca. 5 inH₂O) and a negative pressure (ca. 1 inH₂O) downstream. To maintain a low pressure drop, the filter bag was designed with a mechanical shaking device, which shakes and deforms the bag to break off layers of ash. The ash was collected in a can at the bottom of the filter and stored for future research projects and ash sampling testing. The filter housing and design of the filter bag were completed in-house, while the construction of the filter bag was completed externally.

The visible flame was contained within the first two sections of the combustion chamber (16.7 cm ID) and the third section (37 cm ID) provided sufficient residence time for burnout of larger particles and for the gas composition to become uniform. In order to take detailed in-flame measurements and ensure the flame was contained within a momentum-controlled combustion chamber, the two middle sections were designed and constructed in-house with sampling ports to accommodate both gaseous/ash sampling probes as well as type-K thermocouples lining the inside wall of the refractory along the length of the combustion chamber.
An updated standard operation procedure (SOP) for the laboratory-scale combustor is included in Appendix A. To ensure that the refractory-lined combustion chamber is hot enough to support the ignition and stability of a self-sustained coal flame, the combustor is to be heated up with a 10 kW propane flame for at least two hours. Following the ignition of the coal flame, steady-state gas compositions as indicated by the exhaust CO, O\textsubscript{2} and NO concentrations, could be achieved within 30-45 minutes.

Detailed measurements of pulverized fuel flames on the ~30 kW scale are difficult and limited. In this furnace, experimental measurements are limited to what can be sampled through the discrete measurement ports along the combustion chamber length and the exhaust (Figure 3.1). Methods used in more traditional gaseous flame combustion studies, such as particle image velocimetry (PIV), laser doppler velocimetry (LDV), and even simple temperature measurements are difficult to acquire due to the limited access and harsh environments of pulverized fuel flames. To determine changes in the volatile flame length, centerline species measurements based on methods used in nonpremixed gaseous flames can provide details about the fuel-rich zone.

### 3.2 In-flame gaseous species and particle sampling

Gaseous samples of CO, CO\textsubscript{2} and O\textsubscript{2} were extracted from the combustion chamber using stainless steel nitrogen dilution probes with a 10.2 mm ID dilution tube and a 4.5 mm ID sample tube located at nine ports along the length of the combustion chamber with a typical dilution ratio of 10:1. The samples were dried and filtered before being sent to a continuous emissions monitoring system (CEM) (Horiba, Inc.). Concentrations of O\textsubscript{2} (zirconium oxide cell), CO (nondispersive infrared sensor (NDIR)) and CO\textsubscript{2} (NDIR) were measured. Species measurement
fluctuations between the instantaneous minimum and maximum were up to ±15% in the flame zone and ±5% out of the flame zone. For each experimental point, the values were averaged over five runs to account for daily and day-to-day variations.

Particles were also collected along the centerline of the combustion chamber using an isokinetic nitrogen dilution sampling probe assembly as based on designs Li et al. [53]. The in-flame end of a gas-sampling probe was modified to ensure isokinetic sampling. The probe assembly was attached inline to a vacuum pump and sampling cup arrangement to collect the particles. The location of sampling varied along the centerline depending on the location of the end of the volatile flame. The particle samples were collected and analyzed using thermogravimetric analysis (TGA) (TA Instruments, Inc.) to determine the amount of remaining volatile matter content.

### 3.2.1 Flame length measurements

In gaseous non-premixed flames, the concentrations of CO, CO$_2$, and O$_2$ have been used to indicate the end of the flame [54]. As the end of the gaseous flame is approached, O$_2$ concentrations increase, while CO concentrations decrease to zero. A similar approach is applied in this work to determine the location of the volatile flame. Species measurements of CO and CO$_2$, which can be made accurately, are the most important experimental measurements completed in this work. CO concentrations are high in the fuel-rich side of the volatile flame due high concentrations of volatile fuel and low concentrations of oxygen, but outside the volatile flame the CO concentration decreases to near zero as O$_2$ is available outside the volatile flame to convert CO to CO$_2$. Since some CO is produced from char oxidation, CO concentrations will not go to zero, as they are in gaseous flames, but will asymptote to a finite, near zero value. Thus, the end of the volatile flame can be identified as the location where the concentration of
CO is sharply reduced and begins to asymptote to a near constant value. Rather than consider the CO concentration directly, the CO Fraction, as defined in Equation 3.1, is used because it eliminates the dependence on the dilution ratio of the sampling probes and is a somewhat more sensitive indicator of the end of the volatile flame as it also accounts for the increase in CO$_2$ that occurs due to consumption of CO.

\[
\text{CO Fraction} = \left( \frac{[\text{CO}]}{[\text{CO}]+[\text{CO}_2]} \right) \times 100
\]  

(3.1)

The CO fraction at the end of the volatile flame can also be mathematically estimated based on its relationship to the asymptotic CO fraction after the volatile flame. For example, the end of the volatile flame can be approximated as the location where the CO fraction is within 15% of the asymptotic value. Experimental data for coal and cofired flames with 20 wt.% and 40 wt. % wood waste are shown in Figure 3.2 to illustrate the usage of the CO fraction to measure volatile flame length.

The basic features of the CO fraction profile include the location of peak CO concentrations within the volatile flame zone, which are located between 0.2 and 0.6m for the data presented, and the end of the volatile flame, which lies between 0.9 and 1.5m. Validation and sensitivity of pulverized fuel sub-models for the prediction of the CO fraction within the volatile flame are discussed in Chapter 4 along with further validation of nonpremixed propane flames. More detailed discussions and comparisons of CO fraction profiles and volatile release and reactions are included in Chapter 5, which is focused on volatile flame structure.
3.3 Fuels

Subbituminous Powder River Basin (PRB) coal provided by the local electricity utility and wood waste obtained from a local sawmill were utilized. Proximate, ultimate, and sieve analyses are provided in Tables 3.1 and 3.2. The higher heating value (HHV) is shown on a dry-ash-free (DAF) basis. Some variation in the coal particle size distribution was observed over the course of experiments as indicated by the ranges in the Table 3.2. The wood waste, as received from the sawmill, contained 46 wt.% moisture, as measured by a Hi-Res TGA. The moisture content was reduced to 10 wt.% by exposing the wood waste to laboratory room air for 5 days, after which it was sieved down to < 18 mesh. The average moisture content of the coal was approximately 20 wt.%.

While biomass fuels can be highly variable, some inferences can be made, in general, about the fuel composition characteristics. Compared to coal, biomass fuels have a lower rank with higher volatile matter content and lower fixed carbon. Biomass fuels also have lower heating values,
which means more fuel is needed to maintain a constant heat output. Moisture contents can vary dependent upon the source and location of the fuel. The mean particle size of biomass fuels is typically larger than that of coal. For this study, the mean diameter for coal and wood waste particles is 65 μm and 350 μm, respectively. As mentioned in Section 1.2.4, the fuel-N for biomass fuels also varies. However, the wood waste used in this study contains 0.15% fuel-N, which is significantly lower than the coal.

<table>
<thead>
<tr>
<th>Table 3.1. Ultimate &amp; proximate analyses</th>
<th>Table 3.2. Sieve analysis</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>HHV MJ/kg (DAF)</strong></td>
<td>PRB Coal</td>
</tr>
<tr>
<td>----------------------</td>
<td>------------</td>
</tr>
<tr>
<td>Ash</td>
<td>7.5</td>
</tr>
<tr>
<td>Volatile Matter</td>
<td>43.4</td>
</tr>
<tr>
<td>Fixed Carbon</td>
<td>49.1</td>
</tr>
<tr>
<td><strong>Ultimate Analysis wt. % (dry)</strong></td>
<td>PRB Coal</td>
</tr>
<tr>
<td>Carbon</td>
<td>69.51</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>4.61</td>
</tr>
<tr>
<td>Oxygen</td>
<td>17.02</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0.97</td>
</tr>
<tr>
<td>Sulfur</td>
<td>0.4</td>
</tr>
<tr>
<td><strong>Sieve Analysis wt. % retained</strong></td>
<td>PRB Coal</td>
</tr>
<tr>
<td>18 Mesh</td>
<td>0</td>
</tr>
<tr>
<td>30 Mesh</td>
<td>&lt;0.1</td>
</tr>
<tr>
<td>40 Mesh</td>
<td>--</td>
</tr>
<tr>
<td>50 Mesh</td>
<td>&lt;0.1</td>
</tr>
<tr>
<td>70 Mesh</td>
<td>--</td>
</tr>
<tr>
<td>100 Mesh</td>
<td>1.9-3.2</td>
</tr>
<tr>
<td>200 Mesh</td>
<td>18-29</td>
</tr>
</tbody>
</table>

### 3.4 Chapter Summary

The system improvements that were completed to the experimental system have made it possible to take inflame species measurements and particle sampling. However, these sampling ports can only provide discrete measurements, which can describe the basic features of the flame. Keeping this in mind, an approach utilizing the CO fraction was developed to measure changes in the flame with CFD simulations complementing this data to discover the underlying causes for the changes. The next chapter will discuss the details of the CFD model.
4 Numerical Methods

4.1 Introduction

The use of computational fluid dynamics has been instrumental in furthering our understanding of combustion and flames ranging from fundamental studies of gaseous flames to advanced combustion technologies for industrial-scale flames [55–58]. For flames that can be well characterized using many types of experimental measurements, CFD simulations can be carefully validated and then used for combustor design. On the other hand, when complete validation is not possible, CFD simulations based on established methods and sub-models can be used to complement experimental measurements and provide insight that cannot be obtained from measurements. This work involves the later approach using ANSYS Fluent 13.0, along with limited experiments to understand combustion behavior of pulverized fuel flames where measurements are very difficult. Numerical modeling complements a limited set of experimental measurements to provide insight into coal and biomass interactions within pulverized fuel flames.

Pulverized fuel flames are especially complex, including swirling turbulent flows, high particle loadings, corrosive environment, and high radiative heat transfer. CFD is used in this work to calculate specific quantities that cannot be measured accurately by experiments and are relevant in evaluating the impact of biomass fuels in cofired flames. The goal of using CFD in this work is not to understand the complete flow physics, but instead to focus on certain phenomena within the flame that impact the interaction of biomass particles. While all processes within pulverized fuel combustion need to be accounted for in the model, those processes critical to the interaction of the volatile flame and particles will be focused on and validated to the extent that they can
reasonably predict changes in overall flame behavior.

Flame and particle burning processes have time and length scales that must be considered. Scale is a very important parameter in numerical modeling and determines the type of CFD and the corresponding sub-models used to describe the system. The extent to which the temporal and spatial scales of turbulence are resolved influences the type of CFD that is used and also the amount of computational time needed. Moin and Mahesh [59] mentioned that turbulent flow possesses a mixture of chaos and order and a wide range of length and time scales. However, analytical solutions of turbulent flows do not exist. Direct numerical simulation (DNS) solves the Navier-Stokes equations using known flow variables to completely describe turbulent flow over all time and length scales. This is the most computationally expensive method of CFD. Large eddy simulation (LES) is less computationally expensive than DNS and solves for the large eddy features in turbulent flow, but implicitly solves for the small eddies using subgrid-scale (SGS) models. Lastly, the least computationally expensive method of CFD is Reynolds-averaged Navier-Stokes (RANS). This method assumes the velocity or other instantaneous quantities to be divided into time-averaged and fluctuating quantities, which require closure equations based on turbulent intensity, dissipation, and kinetic energy to solve for the flow field behaviors.

All levels of CFD have been applied to combustion and flames. Depending on what characteristics of the flame are of interest, the type of CFD selected should be a balance between the ability to capture basic features and computational time. For example, if interested in flame stability, particle ignition, or soot formation, DNS or LES would provide the platform for capturing the fluctuating nature of these processes [60,61]. If trying to understand processes in stable flames downstream of the location of stability and after ignition has occurred, then RANS CFD can be used to provide information about the basic features of the system. RANS CFD is
used in this work to see general features of flames and to determine underlying causes of changes in flame structure and emissions.

In the study of pulverized fuel flames, RANS CFD has become a common tool to aid in understanding flame behaviors [55,56,62–64]. Sub-models to capture solid fuel combustion processes for coal are established and have been validated for flames ranging from laboratory-to industrial-scale [65–73]. RANS CFD is also being used to predict flame behavior in advanced coal combustion technologies, including pressurized oxyfuel combustion where limited, if any, experimental data exist [52,53,59–61]. RANS CFD is capable of predicting certain trends and can provide suitable agreement to experiments for conditions close to those where the models have been validated [65,66]. Turbulent pulverized fuel flames are complex systems with many different types of interactions that must be accounted for to make accurate predictions of flames. Fluctuations can also exist in experimental conditions including fuel feed rate, fuel size and composition, and gaseous inlet flow rates. With large model uncertainties and variability in experimental flame conditions, it is not practical to expect accurate predictions of the behavior of pulverized fuel flames.

For example, in a laboratory-scale coal experiment, inlet conditions can vary through the course of the experiments. To minimize variability in the experiments, one large supply of coal and two large supplies of biomass were utilized. The coal had variations in the composition and particle size up to 5%. The biomass has similar size and composition variations. The gaseous inlet flow rates also varied due to downstream pressure fluctuations, which were dependent upon the laboratory HVAC system. These fluctuations can be as large as 10% depending on the day.

The goal of this work is not to predict exact quantities of the flame, but to advance our understanding of the impacts of biomass fuels during cofiring on the volatile flame structure,
which has not been studied before. RANS CFD does have limitations in being able to accurately predict the levels of turbulent interactions, but the solutions are reasonable to show the presence of gross behaviors. RANS CFD simulations can also be quantitatively incorrect, but the existence of interactions with different coals and biomass fuels is known and this work can further elucidate the possibility of how they can interact within the volatile flames.

The focus of the RANS CFD simulations in this work is to model the volatile flame structure of pulverized fuel flames and particle interactions within the fuel-rich zone. RANS CFD simulations are used to complement experimental measurements and provide detailed information. The simulations provide insight and direction, while experiments provide evidence and verification of flame behaviors.

4.2 Summary of model specifications

Table 4.1 includes a summary of the specifications of the model that were chosen for the simulations. The sub-models and particle laws chosen have been utilized by the pulverized fuel community for many types of applications and were applied in scenarios for which they were created. Therefore, no new quantification of error and uncertainty in the conceptual models was completed in this work. However, the sensitivity of specific sub-models critical to the volatile flame region in coal flames are quantified and discussed in the following sections along with experimental validation of propane flames in 2D and 3D for the CO fraction approach. Further validation with coal and cofired flames will be discussed in Chapter 5.
**Table 4.1. Model Specifications for CFD simulations.**

<table>
<thead>
<tr>
<th>Reynolds Average Numerical Simulations (RANS)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Solver</strong></td>
</tr>
<tr>
<td><strong>Discretization</strong></td>
</tr>
<tr>
<td><strong>Pressure-velocity Coupling</strong></td>
</tr>
<tr>
<td><strong>Species &amp; Reaction Mechanism</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>Discrete Phase Model</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>Particle assumptions</strong></td>
</tr>
<tr>
<td><strong>Turbulent-Chemistry Interactions</strong></td>
</tr>
<tr>
<td><strong>Turbulence Model</strong></td>
</tr>
<tr>
<td><strong>Radiation Model</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>Boundary Conditions</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>

**Coal**

<table>
<thead>
<tr>
<th>Devolatilization Model</th>
<th>Chemical Percolation Model (CPD) &amp; Two-competing Rates Model based on TGA data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vaporization onset temperature</td>
<td>650 K</td>
</tr>
<tr>
<td>Char Combustion Model</td>
<td>Multiple Surface Reactions</td>
</tr>
</tbody>
</table>

**Biomass**

<table>
<thead>
<tr>
<th>Devolatilization Model</th>
<th>Two Competing Rates Model based on TGA data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vaporization onset temperature</td>
<td>500 K</td>
</tr>
<tr>
<td>Char Combustion Model</td>
<td>Kinetics/diffusion-limited</td>
</tr>
</tbody>
</table>
Throughout the following sections, the details of the computational mesh and the specific sub-models will be discussed. Within each section, discussions of how models were selected and their impact on the solutions are included.

### 4.3 Grid construction

Grid construction, or domain discretization, for finite volume methods, as is used in ANSYS Fluent, approximates a continuous computational space. The geometry of a physical system is divided into a finite number of control volumes. The construction of the grid is an integral step in the solution process. The quality of the mesh, which includes number, shape, and relative size of the elements, directly impacts the accuracy and stability of the solution and the detail of the physical phenomena that is captured. The computational domain for combustion systems, generally, includes the inlets/outlets and interior of the burner and combustion chamber. The areas of interest to CFD include areas in the physical domain where gases, liquids, and/or heat flow occurs. All other areas can be neglected when constructing the discretized domain.

Gambit 2.4.6 was used to construct the geometry, discretize the domain, and define boundary conditions. Both two-dimensional and three-dimensional domains were utilized, as shown in Figure 4.1. For two-dimensional meshes, common mesh element shapes are rectangles and triangles. Structured (rectangular) mesh elements have regular connectivity, which reduces storage requirements. While, an unstructured mesh allows for the combination of any element (rectangle or triangle) and irregular connectivity, which requires increased storage space for variables in the memory of the solver. Similar descriptions apply for three-dimensional domains utilizing hexahedra, prism, pyramid, and tetrahedral elements shapes. The three-dimensional mesh shown in Figure 4.1b was constructed using a hybrid of structured and unstructured elements. The combustion chamber was meshed using a hexcore meshing
algorithm, which applies several layers of an unstructured mesh near the outside of the combustion chamber and fills the inside with hexahedral elements to reduce the storage requirements.

Figure 4.1. Near burner region (burner and start of combustion chamber) geometry and discretization a) 2D and b) 3D configurations.

A priori knowledge of the important zones in the domain and boundary conditions help to guide grid construction. The location of the flame in the combustion chamber as well as the location of stable flame attachment can help determine boundary conditions and sizes of elements. For stable flames, the location of flame attachment in the near burner region (NBR) is the outer edge of the PO walls. For grid construction, the NBR is composed of the burner and up to several burner diameters downstream in the combustion chamber. This is the location of intense mixing, chemical reaction, particle tracking, heat and mass transfer. The size of the elements in this zone should be small enough to capture steep gradients of important variables within the volatile flame zone.

4.3.1 Grid refinement & independence study

The procedure utilized to estimate the discretization error as well as determine the size of the smallest elements needed for grid independent solutions was based on the Richardson Extrapolation method [57,58]. Solutions computed on three two-dimensional meshes with
varying cell size and grid refinement factors of 1.5 are shown in Table 4.2. The grid refinement study was completed on two-dimensional meshes then applying the appropriate size elements to the three-dimensional mesh. The length of the computational domain for the two-dimensional meshes was selected based on the physical length of the combustion chamber of 2.5m, as shown in Figure 3.1. The length of the three-dimensional mesh was shortened to 1.6m. The length of the flames computed in the grid refinement study and the propane validation study were contained within this region, while ensuring no outlet effects impacted the formation of the volatile flame zone.

**Table 4.2. Computational mesh specifications**

<table>
<thead>
<tr>
<th>Grid Independence Study</th>
<th>2D</th>
<th>3D</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell size</td>
<td>0.095&quot; (2.4mm)</td>
<td>0.042&quot; (1.1mm)</td>
</tr>
<tr>
<td>Number of Cells</td>
<td>37,585</td>
<td>232,000</td>
</tr>
</tbody>
</table>

Converged solutions were computed on the three computational meshes utilizing the following steps and building upon the previous step. For example, the combustion solution is started based on the converged flow field solution.

1. Flow fields (first-order accuracy)
2. Combustion, species, discrete phase model tracking (first-order accuracy)
3. Combustion, species, discrete phase model tracking (second-order accuracy)
4. Radiation modeling (second-order accuracy)
5. NOx species (second-order accuracy)

For each of the coal combustion flame solutions, temperatures, volatile reactions, and oxygen concentrations were monitored at two locations in the NBR and one downstream before the
exhaust for coal combustion flames. From this method and the comparisons of key variables on the three computational meshes, a fine grid convergence index or the numerical uncertainty in the fine-grid solution is reported as 0.5%. Descriptions of the sub-models used to complete these simulations are located in the following sections.

To evaluate discretization uncertainty and to show grid independence for the flames under consideration in this work, Figures 4.2, 4.3, and 4.4 show comparisons of velocity magnitude, volatile release, and temperature.

![Figure 4.2](image)

**Figure 4.2.** Axial velocity profiles for two-dimensional coal flame calculations with varying cell sizes located at a) port 3 (0.23m away from the burner outlet), b) port 7 (0.91m away from burner outlet), and c) port 9 (1.45m away from burner outlet).

In Figure 4.2, the axial velocity profiles located at port 3, which is 22.86cm away from the burner exit, port 7, which is 0.91m away from the burner exit, and port 9, which is 1.45m away
from the burner exit, show good agreement. The maximum differences between the 1.1 mm and the 2.4 mm cell sizes at port 3 are as high as ±14%, but much further downstream at port 9, the maximum differences are around ±7%.

The variable chosen in Figure 4.3 is volatile release that is tracked based on the point of release from the solid particle called the Discrete Phase Model Volatile Source. In all three meshes, the onset and final locations of volatile release are similar, but the magnitudes of release vary up to 75% at the onset location. The fluctuations of volatile release are associated with the particle size distribution of the coal as well as the stochastic tracking model, which introduces random fluctuations to the particle tracking based on the interactions with the turbulent gaseous flow field.

![Figure 4.3. Centerline volatile release profiles for two-dimensional coal flame calculations with varying cell sizes.](image)

Radial profiles of temperature are shown in Figure 4.4. On average, the maximum difference in temperature between the 1.1 mm and the 2.4 mm cell sizes for all port locations is around ±4%. Also, for all cases, by reducing the size from 2.4 mm to 1.6 mm, the maximum difference between the temperatures for all cases is ±1%.
Figure 4.4. Axial temperature profiles for two-dimensional coal flame calculations with varying cell sizes located at a) port 3 (0.23m away from the burner outlet), b) port 7 (0.91m away from burner outlet), and c) port 9 (1.45m away from burner outlet).

The grid size used for the solutions presented for the remainder of this work was the 0.042” (1.1mm) cell size for the two-dimensional simulations. For the three-dimensional simulations, the NBR cell size was 0.042” (1.1mm) growing to 0.25” (6.4mm) at the outlet after the end of the volatile flame to reduce computational time. These solutions were completed maintaining constant sub-models and boundary conditions to obtain the uncertainty associated with the grid. In the following sections, detailed descriptions of the CFD methods and sub-models along with their sensitivity to the formation of the volatile flame zone are included.
4.4 CFD methods

ANSYS Fluent 13.0 was utilized for this work, which uses a finite-volume method solver, to represent partial differential equations (PDE) with a set of algebraic equations solved at discrete locations described by the mesh. Detailed discussions about the forms of the conservation equations, spatial discretization, and segregated solver algorithms chosen for this work are included in Appendix B. Works from Pletcher et al. [77] and Patankar [78] can also provide more detailed information on the finite-volume approach. The following sections will discuss the specific sub-models chosen for pulverized fuel combustion and their sensitivity to the calculation of pulverized fuel combustion.

4.4.1 Convergence criteria

Many factors can influence convergence and the speed to which convergence is reached. A large number of cells in the grid discretization and also complex physics lead to long convergence times. Hardware limitations can also inhibit the speed of convergence, but this discussion will be focused on the limitations occurring within the simulation.

Methods for assessing convergence can vary from one solution to another. The methods used in this work included monitors of the conserved variable residuals and domain monitors created to observe changes of important variables. Scaled residuals, which are reported in Fluent, are defined as the sum of the imbalance between the values at the cell center, the neighboring cells, and the contribution from the source term, which is then divided by the flow rate through the cell. For most terms, this sum should be less than $10^{-3}$ or $10^{-6}$. However, even though conservation equations are satisfied and residuals are converged, the solution may not be correct. Surfaces were created in key locations throughout the domain to monitor velocity, oxygen and volatile concentrations, and temperature. Solutions were considered “converged”
when the variables of interest in the domain monitors and the conserved variable residuals were below the scaled values.

### 4.4.2 Boundary conditions

Boundary conditions were specified based on experiments. The gaseous PO inlet is specified as a mass-flow inlet. The fuel injection was specified on the PO inlet as surface injection with the direction of the flow normal to the boundary. A wall temperature profile was imposed in the model and was based on experimental measurements obtained in the actual combustion chamber.

In two-dimensional axisymmetric solutions, the assumption is that there are no circumferential gradients in the flow. However, swirl flow is experimentally introduced with two tangential inlets leading to gradients in circumferential direction. At high swirl levels, large pressure gradients can drive the flow in the axial and/or radial directions, which defines the amount of swirl in the mean velocity field. To determine the behavior of the flow field without the restrictions of two-dimensional flow, the system was, first, modeled in three dimensions. The flow field from the three-dimensional non-reacting simulation was mapped at key locations throughout the combustion chamber to recreate a similar flow field in two dimensions. Methods by Erdal [79] are utilized to determine the equivalent two-dimensional flow boundary condition (axial, radial, and swirl components) to accurately capture tangential velocity decay and are compared to typical SO boundary condition definition and 3D axial velocity profiles in Figure 4.5.

The axial velocity profiles shown in Figure 4.5 for port 3 highlight the location and flow field behaviors that were the hardest to capture in 2D axisymmetric simulations due to the way
swirling flow is introduced into the combustion chamber. A similar exercise was completed for profiles near the end of the volatile flames away from the NBR, which was shown to have differences of ± 10% between the 2D and 3D solutions. As will be shown in Section 4.3, the flow fields and combustion solutions for propane flames are validated against experimental data with reasonable agreement.

![Figure 4.5](image)

**Figure 4.5. Axial velocity profiles of flow field solutions at port 3 (9” away from the burner outlet) for 3D and varying SO inlet definitions with and without tangential velocity decay.**

The typical 2D SO boundary conditions are applied using axial and tangential components along the same inlet. This method is shown to over predict the velocities. To capture the decay of the tangential velocity component, the axial component is specified on the original inlet location and a new boundary location is specified for the tangential and radial components based on the location of the swirl inlets in the physical system shown in Figure 3.1. This method is shown to have better agreement.
4.4.3 Turbulence and turbulent interactions

Turbulent flow is a contorted stream of high velocity fluid containing numerous mutually interacting, continuously changing eddies or vortices that move with the stream [59,80]. Eddies are responsible for mixing, diffusion, and dissipation of velocity and species throughout the flow and can vary in size and lifetimes. As they evolve throughout the domain and over time, eddies can deform or even break up. In RANS simulations, the equations are time averaged giving rise to new terms known as Reynolds Stresses. These quantities relate to the mean velocity field through turbulent closure models. The governing equations are derived by decomposing the velocity components into time-mean and fluctuating parts and then time averaging the entire equation.

The Reynolds stresses are related to mean velocity gradients utilizing a turbulent viscosity $\mu_t$, turbulence kinetic energy $k$, turbulence dissipation rate $\epsilon$, or specific dissipation rate $\omega$ specified from the turbulent closure models. The complexity of strongly swirling flow fields requires a turbulence closure model that can capture the combination of free and forced vortex flow [81]. The turbulence model chosen for this work is the two-equation eddy-viscosity Shear Stress Transport (SST) $k - \omega$ model [82].

The SST $k - \omega$ model accounts for the transport of turbulent shear stress and gives accurate predictions of the onset and amount of flow separation under adverse pressure gradients [82,83]. Other turbulent closure models that have been used are the family of $k-\epsilon$ models. The $k-\epsilon$ models have been shown to capture the basic features of the turbulent flow features, but have also been known to perform poorly for complex flows involving high levels of swirl and strong streamline curvature [82,84]. The $k-\epsilon$ models are the typical family of models used to capture the fluid mechanics in CFD modeling of pulverized coal modeling [59,60,70–72].
However, the SST k - ω model has been shown to perform better with complex wall-bounded flows and in pulverized fuel cases [70,71,85].

A comparison of the SST k-ω model to the standard k-ε model are shown in Figure 4.6 for the centerline profiles of CO fraction, which is a main indicator for volatile flame length throughout the remainder of this work. It will be shown in later sections that the SST k-ω model is better fit to experimental data. While the CO fraction profile from the k-ε model has similar features, peak CO fraction and location of the end of the volatile flame are shifted and the CO fraction within the flame is under predicted. The level of mixing is not well predicted leading to the decrease in CO species concentrations since the reactions are mixing-limited. The maximum uncertainty in the location of the end of the volatile flame is about ± 14% based on the comparison of these turbulent closure models.

![Figure 4.6. Centerline CO fraction profiles for two-dimensional coal flame solutions with varying turbulent closure models.](image)

### 4.4.3.1 Turbulence-Chemistry Interactions

In RANS simulations, the averaged values of the fluctuating scalars are predicted in turbulent flows. However, instantaneous relationships are used to describe species, density, and
temperature. The averaged turbulent flow field variables are related to the instantaneous values with the turbulent-chemistry interaction model. The Eddy Dissipation Concept (EDC) model [86,87] was utilized due to the fast burning nature of fuels. The eddy dissipation model [87], which is based on the overall reaction rate, is controlled by the turbulence slowly convecting and mixing fuel and oxidizer into the reaction zones where they then burn quickly. The chemical reaction rate is governed by the large-eddy mixing time scale, $\frac{k}{\omega}$. Combustion proceeds whenever turbulence is present ($\frac{k}{\omega} > 0$) [83].

The EDC is an extension of the eddy dissipation model to include chemical reactions in turbulent flows by assuming the reactions occur in small turbulent structures. Combustion within the small scale structures is assumed to occur as a constant pressure reactor, with initial conditions of the current species and temperature in the cells [83]. The reactions proceed over time scales governed by the Arrhenius rates of species creation and destruction and are integrated.

Other options for turbulent-chemistry interactions are finite-rate models and hybrid finite-rate/eddy dissipation models. In the finite-rate models, the chemical reactions control the progression of the flame, while the finite-rate/eddy dissipation model calculates both the mixing and chemical reaction rates and uses the lower rate as the controlling rate. A comparison of the centerline CO fraction for the EDC model and the finite-rate/eddy dissipation model are shown in Figure 4.7. The EDC model will be shown in later sections to have suitable agreement with experimental measurements. The finite-rate/eddy dissipation model can predict the shape of the CO profile, but does not capture the magnitude of the CO and CO$_2$ species within the volatile flame. The combination of mixing and chemical reactions in the EDC model provides a better prediction of species concentrations in the NBR. The finite-rate/eddy dissipation model could
be used to determine the qualitative features of the flame, but based on experimental results is
less accurate for these flame conditions, which is as expected since the conditions of the volatile
flame zone are expected to be mixing-controlled.

**Figure 4.7.** Centerline CO fraction profiles for two-dimensional coal flame solutions with
varying turbulent-chemistry interaction models.

### 4.4.3.2 Turbulence-Radiation Interactions

Just as turbulence is coupled to the chemical reactions, turbulence is coupled to the radiation
heat transfer. In turbulent flames, highly nonlinear interactions exist between chemistry,
turbulence, and thermal radiation [88], which can lead to large fluctuations in temperature and
species concentrations. The spectral radiative absorption coefficient of a gaseous mixture is a
function of both temperature and species, and is, therefore, influenced by any fluctuations
[89,90]. In turn, the heat loss due to radiation influences turbulence. These interactions are
called turbulence-radiation interactions (TRI). Studies have shown that the impacts of TRI can
be as significant as turbulence-chemistry interactions [88]. Turbulence-radiation interactions
can result in higher heat loss due to increased radiative emission, lower temperatures, and
potentially changes in NOx and soot formation [89,91]. The radiative emission has been shown
to be 50-300% higher when accounting for TRI, so that if TRI are not included in the model,
temperatures can be overpredicted by as much as 100°C. Radiatively participating gases such as CO₂ and H₂O, as well as coal/biomass, char, ash, and soot particles all contribute to TRI.

For the flames presented and the approach taken in this work, the volatile flame zone is the focus. While this is the zone of the of flame with high radiation emissions, soot formation, devolatilization and the formation of radiatively participating product gases, detailed TRI will not predicted in this work. If the presence of TRI causes reductions in temperatures throughout the volatile flame region, then local chemistry, devolatilization and volatile combustion may be predicted incorrectly. This would apply to all solutions in this work, but relative comparisons between solutions can still be made. Lower temperatures in the NBR could cause delays in particle heating leading to delayed volatile release and combustion. In pulverized fuel systems, the small particles will be less affected than the large particles. While, this could impact the size of particles that breakthrough the volatile flame and, consequently, the length of the volatile flame, the phenomena would still exist. Therefore, the models and approach presented here can reasonably predict the behavior of volatile flame length and particle breakthrough.

4.4.4 Discrete phase model

Along with solving transport equations for the homogeneous phase, a discrete phase of particles can be described in a Lagrangian frame of reference. The trajectories and mass transfer to and from the particles are computed. The particles occupy a small volume fraction and can exchange momentum, mass, and energy with the gaseous phase. The effect of the discrete phase impacts the continuous phase through two-way coupling and vice versa. The coal and biomass particles were tracked separately using two injections with two different volatile species.

All discrete particles were assumed spherical. The drag force term was based only on the equivalent spherical particle diameter. Intra-particle heat and mass transfer were not included
in the discrete phase particle model. These effects were thought to be of secondary importance for particle sizes considered in this study [92].

The effect of turbulence on particle trajectories is modeled using stochastic methods, which predict the motion of the particle based on the instantaneous fluid velocity including time-averaged mean and fluctuating velocity components. In the Discrete Random Walk (DRW) model, the interaction of particles with the flow is calculated based on the lifetimes of eddies to which the particles pass through. The fluctuating velocity components are calculated based on the local RMS velocity (turbulence kinetic energy) and a normally distributed random number. Typical particle tracks within the laboratory-scale combustion chamber are shown in Figure 4.8 for a coal flame and a 20 wt.% cofired flame.

![Figure 4.8. Particle tracks for a) coal particles and b) biomass particles in a 20 wt.% cofired flame in the laboratory-scale system.](image)

The large biomass particles in the cofired flame in Figure 4.8b are predicted to travel along the centerline only deviating once devolatilization and mass loss has occurred. Large particles burning further downstream were also observed experimentally.
The exchange of momentum between particle and gaseous phase is tracked by the change in momentum of the particle as it passes through each control volume. A sink in the conservation equations represents this change in momentum. The exchange of heat between particle and gaseous phase is tracked in a similar manner by observing the change in thermal energy as particles pass through a control volume. Lastly, mass exchange is also tracked similarly acting as a mass sink in the continuity equation and a source/sink of chemical species in the species conservation equations.

Mass and heat exchanges from the particle to the gaseous phase are governed by laws or relationships that determine the physical processes within the particle. The laws included in this model:

1. Inert particle heating/cooling
2. Droplet vaporization
3. Droplet boiling
4. Devolatilization
5. Surface (char) combustion

The next sections will discuss the specific laws utilized for coal and wood waste. Separate particle injections are tracked for each of the fuels. The particle laws are defined separately based on each of the combusting particles.

4.4.4.1 Coal devolatilization law

Coal particle devolatilization was modeled by the Chemical Percolation Devolatilization (CPD) model [93] and the two-competing rates model [94–96]. The CPD model includes detailed mechanisms of bridge breaking and rearranging of the coal lattice structure, tar evolution, light
gas release, and cross-linking are included. The input parameters for the CPD sub-model were estimated using a chemical structure correlation, with $^{13}$C NMR parameters, based on the ultimate and proximate analysis of the parent coal.

The rate of devolatilization of coal particles described by the two-competing rates model [94] describes mass loss as follows:

$$\frac{m_v(t)}{(1-f_{w,0})m_{p,0}-m_a} = \int_0^t (\alpha_1 R_1 + \alpha_2 R_2) \exp \left( -\int_0^t (R_1 + R_2) dt \right) dt \quad (4.18)$$

Where $f_{w,0}$ is the mass fraction of evaporating material, $m_{p,0}$ is the initial particle mass, $m_a$ is the ash content of the particle, $m_v(t)$ is the volatile yield at time $t$. The two competing rates model incorporates yield factors, $\alpha_1$ and $\alpha_2$, to determine the amount of volatiles released at a low temperature rate, $R_1$, and a high temperature rate, $R_2$. The kinetic rate parameters for coal were derived from Modulated Hi-Res TGA experiments. During the modulated TGA experiments, a heating rate of 20 °C/min ± 5°C was overlaid by a sinusoidal curve with a 200s period, 1.00 sensitivity value, and 6.00 resolution. The pre-exponential factor and activation energy for the two-competing rates devolatilization model were gleaned from these experiments. For the low temperature rate, the pre-exponential factor was $6.0 \times 10^4$ min$^{-1}$ and the activation energy was $1.49 \times 10^7$ J/kmol. For the high temperature rate, the pre-exponential factor was $3.27 \times 10^6$ min$^{-1}$ and the activation energy was $3.2 \times 10^7$ J/kmol. The performance of these models is shown in Figure 4.9 by comparing the centerline CO fraction.
Both devolatilization models are shown to predict very similar profiles for the CO fraction shown in Figure 4.9. However, the CPD model underestimates the CO fraction in the fuel-rich zone of the volatile flame. The prediction of the end of the volatile flame is very similar, while a maximum difference between the two models is about ±14% in the peak CO and peak volatile release zone.

The composition of the volatile matter species are approximated to be one long-chain hydrocarbon species based on the ultimate and proximate analyses [83]. Four global homogeneous reactions were included in the chemical reaction model to capture gaseous volatile reactions as shown in Table 4.3. Separate volatile reactions are included for coal and wood waste with different volatile species, but similar kinetics.
### Table 4.3. Kinetic data for volatile reaction mechanism.

<table>
<thead>
<tr>
<th>Reactions</th>
<th>$A(1/s)$</th>
<th>$\beta$</th>
<th>$E_a$(j/kgmol)</th>
<th>Reaction Orders</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$vol + xO_2 \rightarrow aCO + bH_2 + cN_2$</td>
<td>$2.12E+11$</td>
<td>0</td>
<td>$2.03E+08$</td>
<td>[vol]$^{0.2}[O_2]^{1.3}$</td>
<td>[83]</td>
</tr>
<tr>
<td>$CO + 0.5O_2 \rightarrow CO_2$</td>
<td>$2.24E+12$</td>
<td>0</td>
<td>$1.70E+08$</td>
<td>[CO][O_2]$^{0.25}$</td>
<td>[83]</td>
</tr>
<tr>
<td>$H_2 + 0.5O_2 \rightarrow H_2O$</td>
<td>$1.00E+15$</td>
<td>-1</td>
<td>$1.00E+08$</td>
<td>[H_2]$^{0.25}[O_2]^{1.5}$</td>
<td>[97]</td>
</tr>
<tr>
<td>$CO + H_2O \rightarrow CO_2 + H_2$</td>
<td>$2.75E+09$</td>
<td>0</td>
<td>$8.40E+07$</td>
<td>[CO][H_2O]</td>
<td>[97]</td>
</tr>
</tbody>
</table>

The global kinetic model utilized in this work is able to reasonably predict the end of the volatile flame. Global kinetic models are typically used in the pulverized fuel combustion literature since the reactions are most often mixing-limited and not chemical reaction rate limited. As seen in Figure 4.10, the number of global reactions has very little impact on the structure of the CO fraction profile as well as the critical locations of the peak CO fraction and the end of the volatile flame. This is consistent with the expectation that as long as volatile reactions with oxygen and mixing are reasonably predicted, the location of the volatile flame can also be reasonably predicted.

![Figure 4.10. Centerline CO fraction profiles for two-dimensional coal flame simulations with varying global kinetic reaction mechanisms.](image)
4.4.4.2 Coal char combustion law

For solid particle (char) surface oxidation, a multiple-surface-reaction char model was employed. The following three reactions were assumed to occur as the gas-phase oxidizer diffuses to the particle surface and into the pores. The kinetic data for the char surface reactions is included in Table 4.4.

Table 4.4. Kinetic data for char surface reactions.

<table>
<thead>
<tr>
<th>Reactions</th>
<th>(A(1/s))</th>
<th>(E_a(j/kgmol))</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>(C(s) + 0.5O_2 \rightarrow CO)</td>
<td>2.00E-03</td>
<td>7.90E+07</td>
<td>[98]</td>
</tr>
<tr>
<td>(C(s) + H_2O \rightarrow CO + H_2)</td>
<td>3.19E-01</td>
<td>2.08E+08</td>
<td>[99]</td>
</tr>
<tr>
<td>(1.92E-03)</td>
<td>1.47E+08</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(C(s) + CO_2 \rightarrow 2CO)</td>
<td>1.35E-04</td>
<td>1.36E+08</td>
<td>[99]</td>
</tr>
<tr>
<td>(6.35E-03)</td>
<td>1.62E+08</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Once near the surface, gas is adsorbed and reaction occurs. The heterogeneous reactions can be either controlled by chemical reaction or diffusion. A model of diffusive transport of oxidizer through a porous particle is included. This approach to modeling char burnout has been used throughout the pulverized fuel modeling community, even in advanced oxy-coal combustion applications [21]. While other char combustion models exist, the char burnout zone and the contributions from char were not the focus of this work. All that was needed was a model that would adequately capture char burnout and no other work to validate this model with the laboratory-scale system was performed for this work.

4.4.4.3 Biomass devolatilization law

Biomass particle burning proceeds in three stages: Moisture evaporation, devolatilization and decomposition of lignocellulosic components, and char burnout [100–102]. As the particle heats up, water evaporates and is released from the particle surface and the particle continues to heat up until it reaches the critical devolatilization onset temperature. Devolatilization results in
rapid weight loss as the lignocellulosic components break down. Cellulose provides strength in
the wood fibers, while the hemicellulose acts as a matrix for the cellulose and also acts as a link
between the fibrous cellulose and amorphous lignin [103]. Each component contributes
differently to the overall pyrolysis [104,105]. Hemicellulose decomposition occurs first at lower
temperatures followed by decomposition of cellulose at the higher temperatures. In some cases,
cellulose and hemicellulose decomposition may overlap and decomposition may occur at similar
rates. The last stage of devolatilization is thermal degradation of the lignin, which is generally
composed of high molecular weight compounds. Lignin decomposition typically results in
continuous weight loss at slow rates in the highest temperature regions. The remainder of the
biomass particle burning after devolatilization is similar to that of coal, with the char being
composed of unburnt carbon, ash, and minerals.

For this work, biomass particle burning was treated similarly to coal particles. Within ANSYS
Fluent, the pulverized fuel sub-models are based on coal processes. However, the combustion of
biomass follows similar overall decomposition steps and can be described using analogous sub-
models with inputs based on the biomass characteristics [106]. The rate of devolatilization of
wood waste particles was described using a two-competing rates model [94], which captures the
total decomposition time and rate for all three lignocellulosic components. For the low
temperature rate, the pre-exponential factor was \(7.2 \times 10^{10}\) min\(^{-1}\) and the activation energy was
\(1.4 \times 10^7\) J/kmol. For the high temperature rate, the pre-exponential factor was \(3.27 \times 10^7\) min\(^{-1}\)
and the activation energy was \(7.2 \times 10^7\) J/kmol. The composition of the wood volatiles was
approximated to be one long-chain hydrocarbon species based on the ultimate and proximate
analyses, similar to the coal volatile species.

Another approach to modeling biomass devolatilization that can capture the individual release
characteristics of the lignocellulosic components is distributed activation energy models. This
approach allows the decomposition of hemicellulose, cellulose, and lignin to be modeled in series as three separate volatile release events with variable activation energies [107,108]. For this work, a reasonable estimate of volatile release rate and duration of volatile release was needed to make conclusions about volatile flame length and particle breakthrough. For future work, models with distributed activation energies could provide more quantitative information and identify the limiting component of the biomass volatile release.

### 4.4.4.4 Biomass char combustion law

It has been shown that during wood char oxidation the rates of chemical reaction and gas diffusion through pores are comparable [109]. Therefore, a kinetics/diffusion-limited surface combustion model was chosen based on Baum and Street [110] and Field [111]. In this model the diffusion rates of oxidizer and the kinetics of chemical reaction on the surface are calculated, to determine the limiting process. The particle diameter remains constant but the density can change based on combustion conditions.

### 4.4.5 Radiation model

The Discrete Ordinates (DO) radiation model was implemented for both oxy- [112] and air-fired combustion [113,114]. The radiative transfer equation (RTE) is solved for each cell in the computational domain based on gas emission, scattering addition, and absorption and scattering losses at a position \( \vec{r} \) in a direction \( \vec{s} \) for each cell as shown in Equation 4.19. In the DO method, average intensity is represented by a set of equations over a finite number of ordinate directions [115]. The integrals are replaced by summations over the all ordinate directions to include the \( 4\pi \) of the solid angle.
\[
\frac{dI(\vec{r},\vec{s})}{ds} + (a + \sigma_s)I(\vec{r},\vec{s}) = an^2 \frac{\sigma T^4}{\pi} + \frac{\sigma_s}{4\pi} \int_0^{4\pi} I(\vec{r},\vec{s}')\Phi(\vec{s},\vec{s}')d\Omega'
\] (4.19)

Where \(I\) is the radiation intensity, \(a\) is the absorption coefficient, \(\sigma_s\) is the scattering coefficient, \(n\) is the refractive index, \(T\) is the local temperature, and \(\Phi\) is a phase function integrated over the solid angle \(\Omega\). Incoming and outgoing radiation can move in all directions with parts of a ray included in several cells.

A domain-based Weighted Sum of Grey Gases model (WSGGM) approximates the gaseous absorption in air-fired cases. However, when coal or biomass are combusted in an environment of \(O_2\) and recycled flue gas, the radiative properties can differ from those of air-fired conditions, potentially affecting ignition, stability, temperature, and pollutant formation. Carbon dioxide and \(H_2O\) are radiatively active, and at higher concentrations associated with oxyfuel conditions, the radiative properties of the gas can be altered. Consequently, for oxyfuel combustion, modifications to the absorption coefficient were made using a user-defined function.

An Exponential Wide Band Model (EWBM), which was developed by ANSYS Fluent [116,117], is implemented as a user-defined function to the absorption coefficient. The details of the specific code were not available, but the theory and specifics of validation are included in Krishnamoorthy, et al. [112]. The EWBM uses the integrated band intensity, line-width to spacing parameter, and the bandwidth parameter to describe the total gas band absorptance and to capture the transitions between vibrational and rotational energy states, which provide the greatest contribution to the absorption coefficient.

The effects of radiation are important for particle behaviors. The inclusion of radiation specifically impacts the rate of particle heating, which is a function of both convection and
radiation heat transfer. The effect of the discrete phase on the total radiation was not included. Andersson et al. [117] concluded that the total radiation increases under oxy-fuel conditions namely due to the contribution of the gases. The total particle radiation remains the same in both cases for constant particle loading and temperatures. The oxy-fuel conditions were such that the temperature distribution was similar to that of air-fired cases.

4.4.6 NOx Model

Nitrogen oxides are trace species and their presence does not significantly affect the calculation of the combustion solution or evolution of other species. Therefore, the post-processing NOx model was used. The model for homogeneous NOx formation is divided into two computations for fuel and thermal NO, which includes turbulent interactions for both oxygen and temperature based on the local turbulent fluid dynamics [118]. Prompt NO was not considered.

Nitrogen partitioning in coal particles is based on the methods in [44,118], where 40% is volatile-N and the rest is char-N. Upon being released from the particle, volatile-N reacts with the surrounding gas to form nitrogen intermediates, including NH$_3$ and HCN. For this work, volatile-N is assumed to evolve as 60% NH$_3$ and 40% HCN [119]. Char particles can either produce or consume NO on the surface. NO production from char-N is assumed to form from HCN intermediates [62]. Intermediate species can react with oxygen to form NO and can either remain in the system or be reduced to N$_2$ through reactions with other intermediates or hydrocarbon species. While, nitrogen partitioning of biomass particles is assumed to be 70% volatile-N and 30% char-N [120]. Both volatile-N and char-N is assumed to react to form NH$_3$ intermediates.
Thermal-NO is modeled using the Zel’dovich mechanism, shown in Equations 1.1-1.3 in Section 1.2.2, using the partial equilibrium approach for radical O and OH concentrations.

For the NO data presented in this work, experimental data for flue gas measurements was available as shown in Section 1.2. One step of validation for this work was to predict the flue gas NO concentrations. The NO emissions were shown to have reasonable agreement for air-fired conditions, but not for oxyfuel conditions. However, in both cases the trends were predicted. Therefore, conclusions about the trends of NO emissions and relative changes in NO formation of cofired flames in air-fired and oxyfuel combustion conditions can be made.

### 4.5 Nonpremixed propane flame validation

Propane flame experiments were performed in the same laboratory-scale system to test the capabilities of species measurements along the centerline at the sampling port locations and the ability of the CFD model to predict the flame length of gaseous flames utilizing the CO Fraction. The thermal input was varied from 6-12 kW. The initial approach to locating the end of the flame using the CO fraction was completed by using one sampling probe at a fixed location, while varying the fuel feed rate. With the air flows held constant, the flame length would change based only on the amount of fuel in the system. The plots of CO fraction as function of propane flow rate are shown in Figure 4.11. As shown in the plot for port 7, this curve can indicate when the probe is located inside the flame. When the propane flow rates are low, the probe is sampling downstream or outside of the flame zone. As the propane flow rate increases, the CO fraction will begin to increase when the sampling probe is inside the flame. The goal of these experiments was to simply locate the end of the flame using the CO fraction and not to characterize the entire CO profile.
The fluctuations in CO fraction measurements for the plots shown in Figure 4.11 were very small around ± 4% for all propane flow rates outside the flame and around ± 10% for propane flow rates inside the flame, with the exception of the highest flow rate of port 7. Flames measured at port 7 had the highest propane flow rates. While all flames were turbulent, as the flow rate increased, the frequency and amplitude of flame fluctuations also increased leading to greater variations in species measurements. Inside the flame at port 7, CO fraction variations were measured to around ±20%.

Figure 4.11. Centerline CO fraction experimental measurements in propane flames with varying sampling locations in the combustion chamber and fuel feed rate.
As shown in Table 4.5, the numerical model was able to predict the end of the volatile flame, which is the location where the CO fraction drastically decreases to zero for gaseous flames. As flame length of a gaseous propane flame is controlled by mixing, not kinetics, these results indicate that the fluid mechanics and mixing are adequately represented by the model.

### Table 4.5 Propane flow rates at the end of the flame

<table>
<thead>
<tr>
<th>Port</th>
<th>Experimental (kg/hr)</th>
<th>Predicted (kg/hr)</th>
<th>Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.35</td>
<td>0.38</td>
<td>± 8.5</td>
</tr>
<tr>
<td>6</td>
<td>0.5</td>
<td>0.55</td>
<td>± 10</td>
</tr>
<tr>
<td>7</td>
<td>1.85</td>
<td>1.87</td>
<td>± 1</td>
</tr>
</tbody>
</table>

The temperature profiles for two-dimensional and three-dimensional solutions of propane flames with the end of the flame located at port 5 are shown in Figure 4.12. Based on these propane flame experiments, that the SO boundary conditions needed to include the tangential decay component of the swirling flow to adequately capture the same fluid mechanics in the axisymmetric two-dimensional solutions.

![Figure 4.12. Temperature contours for a) two-dimensional and b) three-dimensional propane flame simulations with the end of the flame located at port 5.](image-url)
The important flow zones that must be predicted are shown in the numerical contours of stream function and velocity vectors colored by axial velocity in the NBR shown in Figure 4.13a and 4.13b. High velocity SO flows from the swirling inlets combined with the low velocity PO flows create a negative flow zone around the exit of the burner. This zone ensures flame stability and increased particle residence times in the NBR. These fluid mechanic features are reasonably captured in the two-dimensional axisymmetric model as was also shown in Figure 4.5.

Figure 4.13. a) Numerical contours of stream function and b) numerical velocity vectors colored by axial velocity for two-dimensional propane flame simulations.

4.6 Chapter Summary

The use of the CFD model alongside experimental measurements offers the opportunity to see details of the flame structure that could not otherwise be measured in the harsh environments of pulverized fuel combustion. While RANS CFD methods have limitations in capturing the
fluctuating and interactive nature of turbulent flames, this approach and the sub-models chosen were shown to approximate the critical processes to volatile flame formation and particle devolatilization with reasonable agreement, such that conclusions about relative trends can be made.

Model sensitivities and validation were presented. The sub-models that have shown the best agreement were utilized in the remainder of the work. Validation of the CO fraction approach using gaseous propane flames showed good agreement, while leading to better methods to define the SO boundary conditions. Further validation of these models with coal and cofired flames will be shown in the next chapters, while explaining the details of the volatile flame structure.
5  The impact of biomass fuels on volatile flame length

5.1 Introduction

Pulverized fuel flames, typically, have two distinct combustion zones: a volatile flame zone and a heterogeneous char burnout zone as shown in Figure 5.1. The length of the volatile reaction zone is important not only for determining the location of maximum temperature and the highest radiative emission, but also for the formation of gaseous pollutants and particulate matter. For example, reduction of fuel-NO relies on homogeneous reactions with nitrogen-containing species would benefit from a longer fuel-rich zone. Furthermore, the volatile reaction zone sets the conditions in the NBR for char burnout and PM formation, which can, consequently, have downstream impacts on loss-on-ignition [121,122], boiler fouling, slagging [123], and ash reuse.

![Figure 5.1. Description of the structure of pulverized fuel flames (picture is a pulverized coal and gas flame courtesy of the LACER lab).](image-url)
The volatile flame zone is characterized by two modes of volatile burning: partially premixed and non-premixed. The fuel is carried to the burner nozzle exit by the PO gaseous stream. Shortly after exiting the nozzle, devolatilization occurs and these volatiles may react with the oxygen that originated in the PO. The amount of oxygen in the PO is typically substantially less than the stoichiometric amount for complete combustion of the fuel, and thus the PO oxygen is consumed by volatiles soon after entering the furnace in a premixed mode of burning. With continued devolatilization, a volatile-rich zone results, leading to a non-premixed mode of volatile burning as the volatiles react with oxygen from the SO. The end of the volatile flame is considered to be the end of the non-premixed volatile burning zone.

Volatile flame structure is influenced by fuel characteristics, fluid dynamics, and burner geometry. In swirl-stabilized burners, flame length decreases as the ratio of swirl to axial momentum (swirl number) increases [50]. Burner design can also impact volatile flame length by altering the residence time of particles in the fuel-rich, near burner zone [124]. Fuel properties that impact the volatile reaction zone include volatile matter content, fuel composition, volatility, moisture content, and particle size [125,126].

5.2 Volatile flame length of a coal flame

The initial approach taken in this work to locate the end of the volatile flame using the CO fraction, which was similar to that used for propane flames in Figure 4.10, was completed by using one sampling probe at a fixed location, while varying the coal feed rate. The plot of CO fraction as function of coal feed rate is shown in Figure 5.2 with flame zones labeled. The end of the volatile flame is experimentally determined to be located at port 6 with a coal feed rate around 2.55 kg/hr. Numerically, the end of the volatile flame is observed at port 6 of a coal feed rate around 2.5 kg/hr within ±2% of the experimental value.
To better understand the overall structure of the volatile flame, the next sections will characterize the centerline CO fraction profiles of flames with constant fuel feed rates for coal and cofired flames. The CO fraction was measured at locations along the length of the flame using sampling probes located at each port in the combustion chamber. In Figure 5.3a, numerical results for CO Fraction and reaction rate of the volatile reaction with oxygen are plotted as functions of distance along the centerline, with the origin corresponding to the exit of the PO. Experimental results for the CO Fraction are also shown by the open circles. Within the flame zone, species measurements fluctuations were much higher than compared to measurements outside the volatile flame zone. Figure 5.3b shows a false color image of numerically-obtained temperature contours for the coal flame.
Figure 5.3. a) Experimental and numerical profiles of CO fraction (−) and numerical volatile reaction rates with oxygen (−−−) along the centerline of a 18 kW coal-fired flame. b) Numerical contours of temperature for the same flame.

Location 1, labeled in Figures 5.3a and 5.3b, coincides with the consumption of oxygen from the PO. Experimental measurements in this zone could not be obtained because the sampling probe disrupted the flow of fuel and PO. Location 2 is inside the fuel-rich flame zone with minimal oxygen and intense volatile release, as indicated by peak CO concentration. Shortly downstream of Location 2 is the maximum reaction rate of volatiles and also the peak temperature, as shown in Figure 5.3a, indicating the volatiles are mixing and reacting with oxygen from the SO. While the quantitative agreement between experimental and simulation is marginal in this zone, the
locations of the peak CO Fraction and the sharp decline are well-matched. Location 3 is the end of the volatile flame where the CO fraction has significantly decreased and the average value is within 25% of the asymptotic value. Once outside the volatile flame, species measurement fluctuations significantly decreased, which also helped determine the end. The end of the volatile flame is predicted by the numerical model within ±3% of the experimental measurements. This location also coincides with the end of significant volatile reaction when a majority of volatiles are released before reaching the end of the flame.

5.3 Volatile flame length during biomass cofiring

Volatile release is affected by many factors, including volatility, volatile matter content, and particle size, which play key roles in shaping the volatile flame. For biomass fuels, the devolatilization process differs from that of coal with higher volatile release rates and lower onset temperatures [126,127]. Coupled with increased volatile matter content, this would suggest that the amount of volatile species should be greater in the near burner zone of the cofired flame. However, biomass particles are also typically larger than coal particles, and the larger size can delay volatile release, leading to a competing effect on the volatile flame length.

Volatile species composition also varies from fuel to fuel. However, the chemical reaction rates for the initial volatile reactions with oxygen are much faster than the turbulent mixing rates for the fuel and oxidizer [128]. Therefore, composition of the volatiles is less important than the rate of volatile release and the mixing rate in the near burner zone for influencing the volatile flame length.
To assess the impact of cofiring, the CO fraction and total volatile reaction rate profiles along the centerline are shown in Figure 5.4 for a cofired flame with 20 wt.% wood waste. The total volatile reaction is the summation of the coal and wood reactions. For this case, the overall volatile mass fraction increased 30% and the volatile release rate increased an average of 24%, both of which should lead to increases in the volatile flame length. However, the 20 wt.% cofired flame has a similar CO fraction profile and volatile flame length compared to that of the coal-only flame.

Figure 5.4. Experimental and numerical profiles of CO fraction (–) and total volatile reaction with oxygen (---) for along the centerline of an 18 kW 20 wt.% cofired flame with wood waste (<18 mesh). The arrow denotes the end of the volatile flame.

When comparing volatile reaction profiles, the end of the volatile flame does not indicate the end of the volatile reaction, as was the case for the coal-only flame. During cofiring, the peak volatile reaction shifts downstream and a significant portion of volatile reaction occurs after the end of the volatile flame. This demonstrates that some of the volatile fuel is not participating in the volatile flame and is, instead, breaking through the volatile flame envelope to react downstream.
5.4 Impact of particle breakthrough on volatile flame length

Breakthrough of the volatile flame by particles before complete devolatilization (herein termed “particle breakthrough”) impacts the non-premixed zone of volatile burning, and thus affects the length of the volatile flame zone. As with gaseous nonpremixed flames, a fuel-rich core is surrounded by oxidizer from the SO. The location of the flame, which is dependent upon local stoichiometry, forms at the interface between fuel and oxidizer [28]. This structure is similar for pulverized fuel flames downstream of the region of consumption of PO oxygen (the premixed zone of volatile burning). The schematics in Figure 5.5a and b illustrate the impacts of particle breakthrough on the volatile flame.

Figure 5.5. Pulverized fuel flame schematics for a) no particle breakthrough of the volatile flame and b) particle breakthrough of the volatile flame. The gray areas represent the char burnout zone.
For flames with no particle breakthrough, as shown in Figure 5.5a, all of the volatile release occurs in the near burner zone and within the volatile flame. Mixing of volatiles and oxygen, with subsequent reaction, leads to the formation of the volatile flame. On the other hand, flames experiencing particle breakthrough have some volatile release occurring downstream of the volatile flame, as shown in Figure 5.5b. Delayed volatile release leads to less fuel available in the near burner region, leading to shorter volatile flame lengths. This is consistent with gaseous non-premixed flame length theory, which states that the flame length is proportional to fuel mass fraction [129]. The volatiles that remain within the particles after breakthrough are released into areas of higher oxygen concentration.

5.5 Biomass particle size

When cofiring biomass fuels, the overall mean particle diameter of the fuel mixture increases as well as potentially forming a bimodal size distribution with one peak for coal and the other for biomass. Large particles have long heating times and high axial momentum, which causes them to travel in the axial direction along their initial trajectory and do not follow the fluid flow streamlines. Both of these effects result in less volatile release in the fuel-rich region of the volatile flame leading to particle breakthrough. Not only are wood particles, on average, double the size of the coal particles used in this study, but they also contain roughly double the volatile matter content. Therefore, particle breakthrough of the volatile flame can potentially lead to significant amounts of volatiles reacting further downstream (Figure 5.4), which can shorten the volatile flame length (Figure 5.5b).

To confirm the presence of particle breakthrough, wood waste was sieved down to < 40 mesh, removing the very large particles. As noted, smaller particles have less axial momentum and shorter heating times. Thus, the smaller particles coupled with the greater volatile matter
content of the wood waste, leads to an increase of volatiles in the near burner zone and a longer volatile flame, as shown in Figure 5.6. Reducing the size of wood particles also leads to reduced particle breakthrough. Therefore, the results of Figure 5.6 confirm that particle breakthrough is present when cofiring wood waste with the original larger particle size distribution and that this leads to a shorter than expected flame length.

![Figure 5.6](image)

**Figure 5.6.** Experimental and numerical profiles of CO fraction (—) and volatile reaction with oxygen (---) along the centerline of an 18 kW 20 wt.% cofired flame with the reduced particle size wood waste (< 40 mesh). The arrow denotes the end of the volatile flame.

Direct experimental evidence of particle breakthrough was found by sampling particles along the centerline near the end of the volatile flame as determined by the CO fraction. To confirm that the sampling probe was located near the end of the volatile flame, samples were taken at ports directly downstream and were observed to have little to no volatile matter remaining. The amount of volatiles remaining in the samples is shown in Table 5.1. For the coal-only or cofiring flames with smaller wood particles (<40 mesh), particle breakthrough is minimal and less volatiles remain. On the other hand, when larger wood particles are present (<18 mesh), high percentages of volatile fuel remain in the particles that are located at the end of the flame.
Table 5.1. Volatiles remaining in particles sampled along the centerline

<table>
<thead>
<tr>
<th>Fuels</th>
<th>Volatiles Remaining (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal</td>
<td>9</td>
</tr>
<tr>
<td>20 wt.% Cofiring</td>
<td></td>
</tr>
<tr>
<td>&lt; 40 mesh wood waste</td>
<td>7</td>
</tr>
<tr>
<td>&lt; 18 mesh wood waste</td>
<td>21</td>
</tr>
</tbody>
</table>

5.6 Cofiring ratio

When increasing the cofiring ratio, there are competing effects leading to a complicated relationship between flame length and volatile release downstream of the flame. When increasing cofiring ratio, both volatile fraction and particle size increase. A greater volatile fraction, in theory, leads to longer flame lengths. Whereas, larger particle size leads to breakthrough of the volatile flame before complete devolatilization, resulting shorter flame lengths. Numerical results for the relationship between particle breakthrough and volatile flame length are shown in Figure 5.7 for cofiring cases with the original wood waste (< 18 mesh). Particle breakthrough of the volatile flame is quantified by the ratio of the integrated area of volatile reaction along the centerline occurs downstream of the end of the volatile flame to the total integrated area of volatile reaction.

![Figure 5.7](image.png)

Figure 5.7. Numerical profiles of particle breakthrough of the volatile flame and volatile flame length of cofired flames with the original wood waste (< 18 mesh).
Increased particle breakthrough occurs at lower cofiring ratios, primarily because of the significant difference between coal and wood particle sizes. At low cofiring ratios, the flame size is governed by coal particles, with large wood particles passing through the flame to devolatilize downstream. At high cofiring ratios, combustion behavior of the wood has a dominant impact on volatile flame length, leading to longer volatile flames and less particle breakthrough, as demonstrated by the CO fraction profiles and volatile reaction rates for a 40 wt.% cofired flame shown in Figure 5.8. The volatile reactions occurring past the end of the volatile flame have significantly decreased and the flame length has increased compared to the 20 wt.% cofired flame shown in Figure 5.4, which is consistent with the trends shown in Figure 5.7.

Figure 5.8. Experimental and numerical profiles of CO fraction (○) and volatile reaction with oxygen (---) along the centerline for an 18 kW 40 wt.% cofired flame with wood waste (< 18 mesh). The arrow denotes the end of the volatile flame.

Figure 5.9 shows the relationship between particle breakthrough of the volatile flame and volatile flame length of cofired cases with the smaller wood particle size (< 40 mesh). Less breakthrough occurs when the wood particle size is reduced, and the volatile flames are longer when compared to the large wood waste cofired in Figure 5.7. Furthermore, the presence of larger wood particles leads to particle breakthrough at any cofiring ratio, whereas with the smaller particles breakthrough ceases to occur at cofiring ratios around 50%.
Figure 5.9. Numerical profiles of particle breakthrough of the volatile flame and volatile flame length of cofiring with small (<40 mesh) wood waste.

The wood waste particle sizes in this study are smaller than what is typical for industrial heating or power generation applications. Average particle sizes can vary in mean diameter between 1 – 3 mm with the largest particles having diameters up to 8 mm [130]. When cofiring wood waste with a particle size distribution similar to industrial sizes, as shown in Figure 5.10, particle breakthrough becomes more significant. For low cofiring ratios, the volatile flame is dictated by the coal volatiles, but as the cofiring ratio increases, the contribution from smaller wood particles increases leading to similar flame lengths. The difference in particle size between wood waste with a particle size distribution typical of industrial applications and coal is much larger leading to increased particle breakthrough and shorter volatile flames. Cofiring ratios greater than 60 wt.% were not simulated due to flame liftoff.
When such large particles breakthrough, the formation of a secondary devolatilization zone can occur further downstream as shown in Figure 5.11. The first peak of the CO fraction originates from the release and reaction of coal volatiles, which is the stabilizing part of the volatile flame zone. The second smaller peak of the CO fraction originates from the downstream release and reaction of biomass particles as they have broken through the primary volatile flame zone.
The first peak of the CO fraction shown in Figure 5.11 is the highest due to greater formation of CO from coal volatiles and the contribution of CO from volatile reactions of small biomass particles. The peak volatile reaction occurs directly downstream of the first peak in CO fraction suggesting that this is the end of the flame zone and reactions occurring past this location originate from particles that have broken through. For this biomass particle size distribution, both coal and biomass particles have broken through leading to significant volatile reaction occurring downstream. These results are consistent with the work of Damstedt et al. [131], who observed large straw particles penetrating the flow fields of the near burner zone, similarly, resulting in a secondary combustion zone. Laux et al. [132] also observed a strong secondary volatile release zone along the burner axis for an industrial scale burner.

5.7 Systematic study of biomass particle size for breakthrough in air-fired and oxyfuel combustion conditions

When particle breakthrough occurs, the thermal/reactive history of the particle is quite different, and this can have adverse effects on NOx formation and LOI [133]. The experimental results previously presented in Section 1.3 showed that NO emissions remained constant as the cofiring ratio increased, even though the wood has much less fuel-N. However, when the wood particle size was reduced, NO emissions decreased in air-fired conditions, but not oxyfuel conditions. The following sections will discuss the conditions for particle breakthrough and the relationship between particle size and combustion environments. This knowledge will be applied to changes in NO formation and emissions during air-fired and oxyfuel combustion in Chapter 6.
The potential for breakthrough of the volatile flame is investigated for 30 kW cofiring flames with monodisperse particle size distributions of wood waste, which is systematically varied. As will be seen, the choice of a monodisperse size distribution allows for a convenient interpretation of the effects of particle size. Previously, volatile flame length was characterized by CO fraction and volatile reaction with oxygen along the centerline. In following sections, the volatile flame is characterized by the location of the high temperature zone, which is controlled by the volatile reaction with oxygen, as shown in Figure 5.12.

![Figure 5.12](image)

**Figure 5.12.** a) Numerical temperature contours and b) volatile reaction rate with oxygen for 30 kW coal flame. Arrows denote volatile flame length.

### 5.7.1 Air-fired flames

Figure 5.13 compares the volatile flame length for three 20wt.% cofired flames with varying wood particle sizes. Figure 5.13a has wood particles with the same size distribution as coal. Figure 5.13b has wood particles with a monodisperse size distribution of 600 μm and Figure 5.13c has wood particles with a monodisperse size distribution of 1 mm.
Locations for decreased centerline temperatures within the volatile flame observed in Figure 5.13b and downstream in Figure 5.12c correspond to the endothermic devolatilization of the wood particles. When comparing Figures 5.13a and 5.13b, the volatile flame lengths are similar even though the wood particle size distributions have changed significantly. Figure 5.13c illustrates that 1 mm wood particles breakthrough and the volatile flame length decreases. This result is similar to what was observed when cofiring industrial size wood waste (Figures 5.10 and 5.11).

![Figure 5.13. Numerical temperature contours for 20 wt.% cofired flames with wood particle sizes of a) the same size distribution as coal, b) 600 μm monodisperse size distribution, and c) 1 mm monodisperse size distribution.](image)

As shown in Figures 5.13b and 5.13c, the devolatilization location of monodisperse wood particles is very pronounced along the centerline. The 600 μm and 1 mm particles are too large to be entrained by the recirculation zone at the exit of the PO and continue along the centerline. Figure 5.14 demonstrates this by comparing the centerline temperatures of coal and cofired flames with uniform particle size distributions. If volatile release occurs within the volatile flame, then the location of peak temperature remains nearly the same as can be seen when comparing the coal flame to the cofired with 600 μm wood particles. On the other hand, for 1
mm wood particles, volatile release occurs downstream leading to a shorter volatile flame and the peak temperature shifted closer to the burner.

![Diagram](image)

**Figure 5.14. Numerical centerline temperatures for 20 wt.% cofired flames with wood waste of varying particle sizes: the same particle size distribution as coal (−), 600 μm monodisperse (−−−), and 1 mm monodisperse (--−).**

By utilizing the endothermicity associated with volatile release, wood particle size may be selected to strategically decrease the peak temperature. For example, Figure 5.15a shows how the centerline peak temperature can be truncated by selecting the wood particle size distribution shown in Figure 5.15b. This size distribution was selected so that the region of devolatilization associated with large wood particles aligned with the region of peak centerline temperature. In this configuration, the wood particles have large axial momentum, thus devolatilization occurs along the centerline. Alternative trajectories for the wood particles are possible with proper burner design [134], and thus, this approach can serve as a method of controlling peak temperatures in select regions of the flame.
5.7.2 Oxy-cofired flames

The effects of wood particle size were also investigated in oxyfuel conditions with an oxidizer composition of 30 vol.% $O_2$/70 vol. $CO_2$, as was used in the experimental work of Section 1.3. The inlet conditions for the air-fired flames shown in the previous section and oxyfuel flames are shown in Table 5.2. The SO flow rate was reduced for oxyfuel conditions, while the PO flow rate was maintained equal to that of air-fired conditions to maintain similar oxygen concentrations in the flue gas.

<table>
<thead>
<tr>
<th>Inlet</th>
<th>Air</th>
<th>Oxyfuel: 30% $O_2$/70% $CO_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Primary</td>
<td>m³/hr</td>
<td>4.4</td>
</tr>
<tr>
<td>Secondary</td>
<td>m³/hr</td>
<td>29</td>
</tr>
<tr>
<td></td>
<td></td>
<td>18.1</td>
</tr>
</tbody>
</table>

The impact of the $O_2/CO_2$ environment and reduced flow rates can be seen by comparing the temperature contours for air-fired conditions (Figure 5.16a) with those of oxyfuel conditions.
(Figure 5.16b). Both cases include 20 wt.% cofiring with wood waste that consists of 600 μm monodisperse particles.

![Temperature contours](image)

**Figure 5.16. Temperature contours for 20 wt.% cofired flames with 600 μm wood particles during a) air-fired and b) oxyfuel combustion conditions.**

Volatile flame length during oxy-cofiring is shorter compared to air-fired conditions. This is a result of the reduced SO flow rate and increased oxygen concentrations, which is consistent with flame length studies for turbulent oxyfuel methane and liquefied propane gas (LPG) flames [135,136]. The same level of swirl was introduced in both cases, which may have also contributed to an overall shorter flame. The volatile flame length is inversely proportional oxygen concentration based on gaseous non-premixed flame length theory [129]. Therefore, for a similar volatile mass fraction, one would expect a shorter volatile flame under oxyfuel combustion conditions.

Delayed volatile release of large wood particles also impacts the volatile flame length of oxy-cofired flames. Under air-fired conditions in the systematic study, volatile release downstream of the volatile flame is not observed for particles size less than 1 mm in diameter. For oxyfuel conditions, breakthrough is observed for wood particle sizes of 600 μm and larger. Therefore,
wood particles can more easily breakthrough the oxyfuel flame leading to devolatilization downstream of the volatile flame.

Devolatilization that occurs outside of the volatile flame in regions of higher oxygen concentration can impact N conversion to NO. The availability of oxygen is a major parameter determining the oxidation selectivity of fuel-N towards NO and N$_2$ [137].

### 5.8 Chapter Summary

This chapter has demonstrated the complex changes that can occur to the flame structure when cofiring two fuels with differing properties, such as wood waste and coal. The volatile flame is composed of two modes of volatile burning: a premixed zone to consume the PO oxygen and a nonpremixed zone, where the remaining volatiles are consumed in a nonpremixed flame with oxygen from the SO. The end of the nonpremixed zone determines the end of the fuel-rich volatile flame zone, which is sensitive to volatile matter content, particle size, and volatile matter release.

Wood waste cofired flames have longer volatile flames compared to coal flames, when most of the volatiles are released in the near burner zone. However, the high momentum and delayed heating of the larger particles can cause particle breakthrough prior to complete devolatilization, leading to shorter volatile flames. At high cofiring ratios, the combustion behavior of the wood waste has a larger impact, leading to longer volatile flames and less particle breakthrough.

Peak particle breakthrough was shown to occur at low cofiring ratios during air-fired combustion for the conditions tested in this work. While, increased particle breakthrough was predicted in oxyfuel combustion conditions.
6  Relationship between volatile flame length & NO formation

6.1  Introduction

The impact of wood waste on flame structure, specifically volatile flame length, has been the focus of this work, primarily because of the implications on NO formation. This chapter focuses on developing an understanding of how changes in volatile flame length impact the production and reduction of NO in the near burner region with an ultimate goal of applying this knowledge to changes in NO emissions.

Figure 6.1 shows NO mole fraction contours in 30 kW coal and cofiring flames with varying wood particle sizes. Net NO formation during cofiring is a consequence of the combined effects of production and destruction. The initial zone of NO production is due to volatile-N reaction with oxygen in the PO. Downstream of this initial production zone, where the NO mole fraction is negligible, corresponds zones of NO destruction. At this location in the combustion chamber, high concentrations of volatile species are released resulting in a fuel-rich, oxygen-depleted zone. NO that has previously formed can interact with nitrogen-containing species to reduce to N₂. NO production is also occurring along the outside of the reduction zones near the walls due to char-N and thermal-NO formation during air-fired conditions.
Figure 6.1. Contours of NO mole fraction for 30 kW a) coal flame and 20% cofired flames with wood particle sizes of b) the same size distribution as coal, c) 600 μm monodisperse size distribution d) 1 mm monodisperse size distribution.

Figure 6.1a shows NO mole fraction contours in a coal flame. High concentrations of NO are produced early in the combustion chamber primarily due to the early formation of HCN from volatile-N. NO production also occurs outside the zone of NO destruction due to char-N conversion and thermal-NO. Since coal, generally, has more char, the downstream formation of NO is greater than when cofiring with biomass, which, generally, has less char. Figure 6.1b shows that when 20 wt.% of the fuel is substituted with wood waste having the same particle size distribution as coal, NO production decreases and the zone of NO destruction enlarges leading to a 30% decrease in NO emissions when compared to the coal case. The lengthening of the NO destruction zone is directly related to the longer volatile flame that results from the increased volatile fraction and minimal breakthrough of biomass particles.

When increasing the wood particle size, as in Figure 6.1c, the size of the initial production zone slightly decreases, but the destruction is more distributed since wood particles are devolatilizing later, resulting in only a 14% decrease in NO emissions over the coal case. An overall reduction
of NO emissions is still observed for this case even though the wood particles are much larger, but devolatilization has occurred within the volatile flame. Lower NOx emissions were also demonstrated in coal flames with varying monodisperse particle size distributions due the small size of the coal particles [138].

For 1 mm size wood particles, NO emissions are nearly the same as the coal case due to devolatilization outside the fuel-rich volatile flame zone into regions of higher oxygen as shown in Figure 6.1d. At the extremes shown in Figures 6.1b and 6.1d, small wood particles enhance NO destruction due to early volatile release and increased volatile fraction, while large wood particles can produce NO downstream of the volatile flame and region of destruction.

### 6.2 Cofiring ratio impacts on NO formation

#### 6.2.1 Air-fired conditions

With increased cofiring ratios, the competing effects of increased volatile fraction and greater quantities of larger biomass particles, also impact NO formation. A summary of NO emissions from air-fired conditions for both experimental and predicted results for varying cofiring ratios of 30 kW flames utilizing <18 mesh wood waste are shown in Table 6.1.

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Fuel Feed rate (kg/hr)</th>
<th>N Content (wt.%)</th>
<th>Experiment [25] NO (ng/J)</th>
<th>Predicted [135] NO (ng/J)</th>
<th>Increase in Experimental N Conversion to NO (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal</td>
<td>4.7</td>
<td>0.98</td>
<td>92</td>
<td>90</td>
<td>-</td>
</tr>
<tr>
<td>10 wt.% Cofiring</td>
<td>4.8</td>
<td>0.90</td>
<td>89</td>
<td>90</td>
<td>3</td>
</tr>
<tr>
<td>40 wt.% Cofiring</td>
<td>6.0</td>
<td>0.64</td>
<td>89</td>
<td>83</td>
<td>14</td>
</tr>
</tbody>
</table>

The “N content” listed in Table 6.1 is the overall fuel-N of the fuel mixture, which decreases during cofiring. In order to maintain the same thermal input, the overall fuel input is higher for
cofiring cases since the heating value of the wood waste is lower than that of coal. Given the much lower nitrogen content of the wood waste, one might expect that the NO concentration in the flue gas would be less when cofiring. Nonetheless, the NO emissions remained nearly constant. Consequently, the conversion of N to NO is found to increase with cofiring ratio. For low cofiring ratios, the percentage of biomass particle breakthrough was shown to reach a maximum (Figure 5.7). However, the total percentage of biomass particles and their corresponding fuel-N are low leading to a small increase in N conversion to NO. However, at higher cofiring ratios, breakthrough was shown to decrease, but greater quantities of large particles exist leading to increased N conversion to NO.

With ANSYS Fluent, one is able to evaluate the contribution of thermal-NO individually. Analysis of these numerical results indicates that changes in thermal-NO during cofiring do not significantly contribute to the increases in N conversion during air-fired conditions.

### 6.2.2 Oxyfuel conditions

As was observed in Section 5.7.2, the critical size for wood particle breakthrough before complete devolatilization occurs at smaller particle sizes during oxyfuel combustion. This leads to greater volatile release in regions of higher oxygen concentration, which was shown to increase net NO formation. Table 6.2 summarizes NO emissions for oxyfuel combustion for both experimental and predicted results with varying cofiring ratios for 30 kW flames utilizing <18 mesh wood waste.
### Table 6.2. Summary of NO emissions from 30 kW oxyfuel conditions

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Fuel Feed rate (kg/hr)</th>
<th>N Content (wt.%)</th>
<th>Experiment [25] NO (ng/J)</th>
<th>Predicted [139] NO (ng/J)</th>
<th>Increase in Experimental N Conversion to NO (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal</td>
<td>4.9</td>
<td>0.97</td>
<td>59</td>
<td>43</td>
<td>-</td>
</tr>
<tr>
<td>10 wt.% Cofiring</td>
<td>4.8</td>
<td>0.90</td>
<td>60</td>
<td>44</td>
<td>14</td>
</tr>
<tr>
<td>40 wt.% Cofiring</td>
<td>6.0</td>
<td>0.64</td>
<td>62</td>
<td>46</td>
<td>32.5</td>
</tr>
</tbody>
</table>

Comparing the experimental results in Tables 6.1 and 6.2, decreased NO emissions are observed for all oxyfuel combustion cases, which can be attributed to the elimination of thermal-NO. The numerical results for NO emissions are consistently lower than that of the experimental measurements; however, the trends are reproduced. Similar to air-fired cases, as the cofiring ratio increases the NO emissions remain relatively constant in oxyfuel conditions. Increased N conversion to NO is not only a result of the shorter volatile flames, but also due to the increased breakthrough of particles devolatilizing downstream of the volatile flame, when compared to air-fired conditions. When cofiring higher percentages of wood waste in oxyfuel conditions, a greater quantity of large particles devolatilizes outside the volatile flame leading to even greater NO conversion.

### 6.3 Other considerations for increased NO emissions

Another factor that could impact NO emissions during oxyfuel combustion is the PO stoichiometric ratio. Skeen [26] showed that when PO oxygen concentrations exceed 30 vol.%, increased NO emissions resulted. At this oxygen concentration the PO stoichiometric ratio reaches some critical value. Therefore, since PO oxygen concentrations were kept below 30 vol.%, changes in PO stoichiometric ratio would not contribute to the change in NO emissions observed.
6.4 Chapter Summary

Large biomass particle breakthrough of the volatile flame before complete devolatilization resulted in increased nitrogen conversion to NO, which is consistent with earlier experimental results. Impacts on volatile flame length and NO formation were magnified at higher cofiring ratios.

Nitrogen oxide formation during oxyfuel combustion combined with biomass cofiring was evaluated. As was previously shown, oxyfuel combustion flames compared to air-fired flames have shorter volatile flames due to elevated oxygen concentrations, decreased flow rates, and increased swirl. These combustion environment changes resulted in flame structure impacts that were detrimental to NO formation. Due to the smaller flame length, the breakthrough of large biomass particles occurred at smaller diameters. Therefore, a larger number of particles released volatiles and volatile-N into areas of higher temperature and oxygen concentrations, leading to increased nitrogen conversion to NO. However, overall NO formation during oxyfuel combustion is reduced compared to air-fired conditions due to the elimination of the thermal-NO mechanism.
7 Criteria to predict particle breakthrough of the volatile flame

7.1 Introduction

Pollutant formation is one of the many reasons as to why understanding the volatile flame in solid fuel combustion is in important. The volatile flame sets the conditions for which particles devolatilize, char burnout proceeds, heat is transferred to boiler tubes, and the flame remains stable and attached to the burner. However, within a stable flame, many properties are fluctuating and changing over time and space within the combustion chamber. In previous sections, experimental measurements were instantaneous values averaged over many runs and numerical values were averaged based on RANS assumptions. The nature of a solid fuel flame is highly turbulent with fluctuations occurring in the combustion and particle burning processes.

The fluctuating nature of turbulent solid fuel flames is investigated focusing on the relationship between particle behaviors and the gaseous volatile flame. During particle conversion, fuel size is expected to have noticeable effects primarily due to the coupling between heat and mass transfer [140]. Scaling methods are utilized to develop a simple model to evaluate the potential for biomass particle breakthrough in solid fuel flames. While the previous chapters have shown that this phenomena can occur utilizing laboratory-scale experiments and CFD modeling, scaling methods and based on the properties of the flame and particle devolatilization process can provide a means to determine the presence of particle breakthrough. This analysis is a work-in-progress with plans for completion and publication in Spring 2013. The concept and current progress is presented with a final section of future work.
7.2 Basic Approach

The volatile flame region is dependent upon the coupling between devolatilization of gases from the solid fuel particles and their associated combustion reactions leading to the formation of flame region that behaves similar to a gaseous flame. The volatile gases are the fuel source for the flame, but the heat transfer from the gaseous oxidation reactions is needed to enable devolatilization and speed up particle heating. Even though volatile flame formation and particle devolatilization processes are coupled, they can be calculated separately in order to predict particle participation in the volatile flame using the following methods and assumptions:

1. Calculate the length and time to the end of the gaseous volatile flame. For this calculation, the maximum amount of volatiles entering the system is assumed to estimate the gaseous flame length, which will implies no breakthrough and the longest length that the gaseous flame could achieve. The length will be coupled with the mean flow field velocities to determine the residence time within the volatile flame zone.

2. Determine the time scale for particle interactions and devolatilization. For the initial approach, only biomass particles are considered. The previous analysis showed breakthrough to occur primarily due to biomass particles.
   a. Determine mixing and ‘cloud’ parameters for group combustion interactions. The solid fuel particles interact with the turbulent flow field and each other, which can impact the time for volatile release.
   b. Calculate the time for volatile release of particles of a given diameter. The time for devolatilization of a single particle includes steps for particle heating, release of volatiles, and diffusion away from the particle. The impacts of ‘cloud’ combustion and particle interactions will be combined here to calculate a total devolatilization time.
3. Compare gaseous flame and particle devolatilization time scales utilizing on a new dimensionless number to determine the presence of particle breakthrough.

The following sections will outline the details of the flame structure and particle devolatilization processes occurring within the volatile flame zone as well as the approach to calculating the length and time scales of gaseous flames, mixing and ‘cloud’ interactions, and particle devolatilization.

### 7.3 Structure and processes of volatile flame formation in solid fuel combustion

As was previously described in Figure 5.1, the volatile flame has two zones of volatile burning. The partially premixed volatile burning zone is located at the base of the flame where volatiles are rapidly mixed with PO oxygen and reacted away. The PO oxygen concentration is well below stoichiometric consuming only a small fraction of the total available volatiles. Therefore, a majority of volatiles burn downstream in the nonpremixed zone, which will be the focus of this analysis. Particle breakthrough, ultimately, impacts the volatiles available for nonpremixed burning. Figure 7.1 illustrates the complex processes that occur within the near the burner region to form the volatile flame.
Figure 7.1. Schematic of flame and particle processes occurring in the near burner zone at levels of (a) nonpremixed turbulent gaseous flame, (b) eddy mixing and entrainment of gases and particles, (c) group combustion of particles within eddies, and (d) single particle devolatilization leading to the release of volatile gases from the particle.

7.3.1 Nonpremixed turbulent gaseous flame

The basic principles of turbulent nonpremixed flames combine turbulent jet mixing theory with diffusion flame correlations [141–143]. In nonpremixed flames, the fuel and oxygen initially enter the combustion chamber separate, to which fuel and oxygen diffuse towards each other creating highly exothermic combustion reactions at the interface. However, in turbulent jet flames, the interface between fuel and oxygen is no longer well-defined, but instead is controlled by entrainment due to turbulent mixing and eddy formations leading to the fluctuating nature of the flame, as shown in Figure 7.1a. Another level of complexity in gaseous flame formation is when the fuel species are initially embedded in the solid structure of a particle and must be liberated to sustain the gaseous fuel needed for combustion reactions. Volatile flame formation is a coupling between the particle pyrolysis processes and turbulent mixing. Once volatiles have
been released from the solid particles, volatile flame combustion is assumed to proceed similar to gaseous turbulent nonpremixed flames. Therefore, further understanding of the particle interactions with the turbulent flow field and the gaseous combustion process is needed to predict the presence of particle breakthrough before complete devolatilization.

### 7.3.2 Turbulent mixing

Turbulent convection mixes fuel and oxidizer based on macroscopic mixing, which is a function of inlet velocities, combustion chamber geometry, and gaseous compositions. Small scale molecular mixing completes the mixing process to ensure chemical reactions take place. Mixing in turbulent flows is characterized by the formation of eddies which create the velocity fluctuations and instabilities that are modeled by Reynold Stresses imposed over a mean velocity field. Figure 7.1b illustrates the eddy interactions with the flame. The size and lifetime of eddies varies throughout a combustion system. Smaller eddies dominate the flow in the near burner region due intense mixing of the PO and SO gases. While larger eddies dominate the flow field downstream as the flow slows and the level of mixing decays. The largest eddies in the system are based on the integral length scale, which are limited by the geometry of the combustion chamber [144]. The largest eddies, also called the energy-bearing eddies, contain most of the kinetic energy of turbulent motion, which “cascades” down to smaller scale eddies [145]. The “cascade” of kinetic energy breaks up eddies into smaller and smaller length scales until a level is reached where the scale is small enough for molecular diffusion and viscous dissipation to control the concentration fluctuations [144], known as the Kolmogorov length scale, which is the smallest scale in turbulent motion.

Turbulent eddies impact the transport and pyrolysis behaviors of the solid fuel particles. The interaction of particles and turbulence is illustrated in Figures 7.1b and 7.1c. For systems with a
dilute particle phase, dense regions or voids of particles are formed by the action of eddies acting on the particles, which is called preferential concentration [146]. Maxey & Corrsin [147] also noted that particle positions may be strongly correlated to motions of turbulent eddies. Preferential clustering of gaseous fuel can also occur, which contributes the fluctuating nature of turbulent flames. This behavior is captured utilizing flamelet approaches [148], but will not be a focus for this work.

The behavior of particles in the flow field, and, consequently, the potential for preferential concentration, can determined based on the Stokes number as defined in Equation 7.1.

$$\text{Stk \#} = \frac{\rho_p d_p^2}{18 \mu}$$  \hspace{1cm} (7.1)

Small particles with low Stokes Numbers follow the fluid parcels of the flow and do not remain entrained in the eddies. While, very large particles with high Stokes Numbers, do not respond fast enough to remain entrained. Larger particles are only affected by the motions of larger energy-bearing eddies and are, generally, the particles most at risk for breaking through the volatile flame before complete devolatilization. Particles with intermediate Stokes numbers will remain entrained in the turbulent vortices and also in convergence areas between vortices with low vorticity and high strain rates [149].

This work focuses on the influence of particle size of spherical particles on volatile release and interactions in the turbulent flame. However, biomass particles can also be non-spherical. The coupling of particle orientation, rotation, and translation are also connected to the motion of the flow structures [150]. Lu et al. [151] showed that both particle shape and size can affect the product yield. While the development of this simple model and dimensionless number is a
work-in-progress, the basic concepts and important variables are included here. Other aspects, such as particle shape, can be addressed in the next phase of development.

7.3.3 Particle devolatilization process

The amount of solid fuel particles in a system is, generally, based on the higher heating value and the mass flow rate needed to maintain a certain power output. In a mass flow of solid fuel particles, there can be on the order of millions of particles entering the system [152]. Therefore, the particles will not behave as isolated particles; rather can be treated as an aggregate of solid fuel particles with modified behaviors due to the presence of other particles. Interactions between particles can alter the drag coefficient, flow field streamlines, ignition delay depending on the denseness of particles, competition for heat and oxygen, and gaseous volatile distribution around the particles [153]. Solid fuel particle burning is a ‘cloud’ or group combustion process rather than a ‘single particle’ process [154]. The term ‘cloud’ refers the clustering of groups of particles, usually much more than 10 [153]. The particles are assumed to form ‘clouds’ based on the sizes of turbulent eddies.

Within the ‘cloud’, heat and mass transfer between the gases and the particles occurs, followed by particle pyrolysis, which based on the single particle models, as illustrated by Figures 7.1c and 7.1d. The focus of this work is on the availability of volatiles. Therefore, burning processes leading up to devolatilization will only be considered. It is assumed that once the volatiles have released from the particle and are transported from the ‘cloud’, that oxidization reactions occur rapidly.
7.4 Flame and particle devolatilization time scales

Utilizing the processes outlined in Section 7.2 and Figure 7.1, details of the flame and particle devolatilization estimated time and length scale calculations will be discussed.

7.4.1 Prediction of nonpremixed turbulent flame length

Nonpremixed flames, as is shown in Figure 7.1a, have fluctuating and almost bushy edges due to the presence of turbulence, which impacts the length of gaseous flames. At high flow rates, increased turbulence leads to increased mixing and eddy formation, which promotes oxidizer entrainment and shorter flames [155]. At high levels of turbulence, flame length remains nearly constant independent of flow rate increases. The length of nonpremixed turbulent flames depends on four main factors [28]:

- Initial jet momentum flux and buoyant forces acting on the flame
- Stoichiometry
- Ratio of nozzle fluid to ambient gas density
- Initial jet diameter

Based on correlations of a non-dimensional flame length and the flame Froude number, Delichatsios [129] found that the nondimensional flame length remained constant for momentum-controlled flames. The nondimensional flame length is defined as

\[
L^* = 23 = \frac{L_f s}{d_j \rho_e \rho_\infty^{1/2}} \tag{7.2}
\]
where \( L_f \) is the actual flame length, \( d_j \) is the initial jet diameter, \( \rho_f / \rho_\infty \) is the density ratio between the nozzle fluid to ambient gas density. For the flames studied in this work, “ambient” is assumed to be gases in the combustion chamber that the PO contacts with when exiting. The stoichiometric mixture fraction is defined as

\[
f_S = \left( 1 + \frac{y_{F,0}W_0}{y_{O,0}W_F} \right)^{-1}
\]  

(7.3)

where \( y_{i,0} \) is the mass fraction of fuel (F) and oxidizer (O) at the inlet, \( W_i \) is the molecular weight, and \( v_i \) is the stoichiometric coefficient. From these equations, the actual flame length can be solved.

The residence time to the end of the volatile flame is based on the velocity of the mean flow field, which is calculated using the inlet conditions of the PO and SO based equations by [49] for the axial decay for a double concentric jet,

\[
\frac{v_{o,t}}{u_m} = K_u \frac{x_c}{D_c} + C
\]  

(7.4)

where \( U_m \) is the mean velocity at \( X_c \), which is the distance in the combustion chamber, \( D_c \) is the equivalent diameter of combined double concentric jets based on the densities and mass flow rates of the PO and SO, \( C \) is a function of PO and SO velocity ratio. \( K_u \) is the mixing parameter for swirling jets, and \( S \) is the swirl number.

\[
K_u = 0.147 + S^2
\]  

(7.5)
7.4.2 Group combustion for solid fuel burning

Figure 7.1c illustrates the physical approach to ‘cloud’ combustion of solid fuels. Methods based on group combustion analyses by Annamalai et al. [152,153] are used to estimate the time scale of particle pyrolysis entrained in ‘clouds’ the size of the turbulent eddies. Most of the mass of particles is in the range of intermediate Stokes numbers, which means these particles will be become entrained within turbulent eddies. As an initial assumption, the ‘cloud’ size is based on Kolomogorov length scale eddies. Ultimately, since coal and wood waste have a size distribution, a distribution of eddies can be weighted to entrain all sizes of particles.

For particles grouped in the ‘cloud’, heat transfer from the mean flow field into the center of the ‘cloud’ occurs based on the time scale of

\[ t_{th,c} = \frac{R_c^2}{\alpha_g} \]  

(7.6)

where \( R_c \) is the radius of the ‘cloud’ and \( \alpha_g \) is the thermal diffusivity of the gas within the ‘cloud’. This time scale is the limiting factor in determining the total time for volatile release around \( \sim 600 \) ms. Conditions similar to the near burner fuel-rich region are assumed for the gases inside the ‘clouds’. For the initial analysis, heat transfer from the ambient is assumed to be fast compared to the total transport between the gas and the particles within the ‘cloud’.

As the particles heat up, the heating rate is controlled by diffusion of heat to the center of the particle and the characteristic time needed to heat up the mass of the particle. While these process can occur simultaneously, the time scales are, generally, on the same order of magnitude around \( \sim 100 \) ms for an average biomass particle. Time for diffusion to the center of the particle is
\[ t_d = \frac{d_p^2}{4\alpha_p} \]  

(7.7)

where \( d_p \) is the particle diameter and \( \alpha_p \) is the thermal diffusivity of the particle. The time required to heat the particle mass is defined by

\[ t_p = \frac{d_p^2 \rho_p C_p}{6\lambda_p Nu} \]  

(7.8)

where \( \rho_p \) is the particle density, \( C_p \) is the particle specific heat capacity, \( \lambda_p \) is the particle thermal conductivity, and \( Nu \) is the Nusselt number assuming heat transfer by conduction from a spherical surface to a stationary, infinite medium around the surface.

### 7.4.3 Single particle devolatilization

As solid fuel particles heat up, water evaporation occurs at 100°C (373 K), which is only a phase process where water leaves the surface once vaporized. The particle will continue to heat up to the devolatilization onset temperature, which is determined based on the material characteristics. The onset temperature is the temperature at which devolatilization begins. Devolatilization, is a decomposition process, which involves the change of chemical composition and physical phase change leading to gaseous volatiles leaving the solid particle surface [156]. The time scale for devolatilization is defined as

\[ t_{pyr} = \frac{\ln(2)}{k_v} \]  

(7.9)
where $k_v$ is the rate of devolatilization based on single rate kinetics. While many detailed models exist, single order devolatilization models provide a good initial estimate.

$$k_v = B_v \exp (-E_v / (R_u T_p))$$  \hspace{1cm} (7.10)

where $B_v$ is the pre-exponential factor, $E_v$ is the activation energy, $R_u$ is the universal gas constant, and $T_p$ is the temperature of the particle. The temperature of the particle influences the time for devolatilization, but volatiles release is fast compared to the particle heat up times on the order of ~ 1 ms.

Lastly, once gaseous volatiles have released they build up on the particle surface. As the volatile generation continues, the gradient of fuel species on the surface becomes greater than the concentrations in the gases surrounding the particle. The volatiles will then diffuse away from the particle into the ‘cloud’. Once in the ‘cloud’, it is assumed that the volatile fuel is available for oxidation reactions. The time for diffusion away from the particle surface can be defined by

$$t_{d,p} = \frac{l^2}{4D}$$  \hspace{1cm} (7.11)

where $l$ is the interstitial spacing between particles within the ‘cloud’ and $D$ is the diffusion coefficient of the gases. The distance of volatile diffusion away from the particle is a function of the spacing between particles in the ‘cloud’, the particle diameter and the ‘cloud’ diameter. The time for volatile species diffusion away from the surface to the particle is on the order of ~20 ms.
7.5 Dimensionless number for particle breakthrough prediction

A comparison of flame and particle time scales determines the presence of particle breakthrough of the volatile flame before complete devolatilization by coal or biomass particles. The gaseous flame length is calculated based on the volatile fraction of the fuel entering the combustion chamber. The flame time scale, \( t_{\text{flame}} \), is the residence time within the length of the volatile flame, which is defined as

\[
t_{\text{flame}} = \frac{L_f}{u_m}
\]  

(7.12)

The time scale for particle devolatilization of a single particle size within the size distribution for a given fuel is the summation of the group combustion heat transfer time and the single particle pyrolysis times, which is defined by

\[
t_{\text{particle}} = t_{\text{th.c}} + t_d + t_{\text{pyr}} + t_{d,p}
\]  

(7.13)

To determine the presence of particle breakthrough for a given particle size, the time scale of maximum flame length is compared to the time scale of particle pyrolysis within the flame through a dimensionless number called the Volatile Flame Number, which is defined as

\[
VF# = \frac{t_{\text{flame}}}{t_{\text{particle}}}
\]  

\[\begin{cases} 
\geq 1, & \text{No breakthrough} \\
< 1, & \text{breakthrough}
\end{cases}
\]

(7.14)

\( VF# = 1 \) corresponds to the flame time equaling the total particle pyrolysis time. Physically, this is the location in the combustion chamber when the volatile flame has ended and only particles
that release volatiles prior to passing through this location are included in the volatile flame. If the devolatilization time exceeds the flame time, then breakthrough occurs and $VF# < 1$. Whereas, if the flame time exceeds the particle pyrolysis time, then $VF# > 1$ with no breakthrough.

At the point of breakthrough, $VF# = 1$, the critical size of particles that breakthrough before complete devolatilization can be determined based on the information shown in Figure 7.2. The critical size for particle breakthrough is calculated by setting the time within the gaseous flame zone, $t_{flame}$, equal to the particle devolatilization time, $t_{particle}$. For this analysis, the flame time, which is calculated based on the total amount of volatiles in the system, varies for each cofiring ratio. The heat transfer into the ‘cloud’ and the diffusion of volatiles away from the ‘cloud’ depend on the eddy size, but not particle size. The time for devolatilization (i.e. volatiles to leave the surface of the particle) is based on the properties of the fuel. Therefore, the time for particle heating, which is a function of particle size, can be solved for, leading to the critical particle size diameter for breakthrough.

![Figure 7.2](image_url)

**Figure 7.2.** Numerically predicted critical size of biomass particles to breakthrough the volatile flame before complete devolatilization for $VF# = 1$ of 18 kW cofired flames with varying % biomass.
For low cofiring ratios, the critical size of biomass particles to breakthrough reaches a minimum size around 250 μm. This is also around the particle size where the combustion rate begins to be influenced by size and shape [69] potentially leading delays in volatile release. As the volatile flame length and cofiring ratio increase, larger biomass particles participate in the volatile flame reducing particle breakthrough, which agrees with the results in Section 5.7. For the coal flame, the critical size for breakthrough is larger than 99.98% of the particles based on the particle size distribution given in Table 3.2. Therefore, breakthrough is negligible in coal flames.

Based on the VF#, the following parameters can be varied to prevent particle breakthrough of the volatile flame:

- Turbulent mixing, which impacts the size of particles entrained into ‘clouds’. The heat transfer through the ‘cloud’ to the particles is a limiting step in volatile release due to the \( R_e^2 \) dependence.
- Particle size, which has a \( d^2 \) dependence on particle heating.
- Available volatile fraction, on which the volatile flame has a linear dependence.
- Velocity of the mean field, which includes swirl and momentum ratio of the PO and SO. This velocity has a direct impact on the length of the gaseous flame.

As mentioned, this is a work-in-progress with plans for completion and publication in Spring 2013. While this preliminary analysis is promising, future plans for other considerations in VF# include:

- Further comparison with experimental and numerical data to refine the equations and assumptions made.
• Inclusion and further investigation of the range of turbulent eddies to calculate a $t_{\text{particle}}$ that is representative of all particles in the distribution.

• Assess how to include the impacts of particle shape in turbulent eddy interactions and the particle heating times.

• Use $\text{VF}#$ to quantify the amount of particle breakthrough similar to the CFD analysis in Section 5.7.

7.6 Chapter Summary

A simple model was developed utilizing scaling methods to determine the conditions for particle breakthrough of the volatile flame before complete devolatilization. The volatile flame region is dependent upon the coupled processes of the gaseous flame and particle devolatilization. The gaseous flame length can be estimated based on momentum-controlled gaseous nonpremixed turbulent flames. While the particle devolatilization process, is a function of ‘cloud’ combustion particle interactions, particle heating and volatile release. By comparing the time scales for the gaseous volatile flame and particle devolatilization, a dimensionless number, $\text{Volatile Flame} #$, can be used to determine the presence of and the critical diameter for particle breakthrough. The minimum critical particle size for breakthrough occurs for cofiring ratios around 10 wt.%, which is consistent with previous results showing increased breakthrough at lower cofiring ratios.
8 Conclusions & Recommendations

8.1 Conclusions

With impending RPS and CO$_2$ legislation, the use of biomass fuels to supplement coal combustion in existing PC boilers has the potential to become important for the large-scale power generation sector, especially in regions, which heavily rely on coal-fired power to meet demand. However, the existing burners and boilers have been optimized for coal, so the direct substitution of biomass can lead to undesirable burner performance and flame length, which could negate some of the potential benefits of cofiring. As a result of this work, an understanding of the volatile flame region during cofiring based on experimental, CFD, and detailed analyses of flame behavior methods ensures current combustion standards and pollutant emissions can be maintained and/or improved.

Volatile flame structure changes that occur during biomass cofiring leads to volatile release downstream of the fuel-rich region impacting both flame length and NO formation. The volatile flame is composed of two modes of volatile burning: a partially premixed zone, which only consumes a small amount of the total volatiles, and a nonpremixed zone, where the majority of volatiles are consumed in a nonpremixed flame with SO oxygen. The end of the nonpremixed zone, which coincides with the end of the volatile flame zone, was successfully measured using experimental measurement techniques based on gaseous flames.

Cofiring with wood waste results in longer volatile flames compared to coal flames, when most of the volatiles are released in the near burner zone, due to their higher volatile fractions. However, the higher momentum and delayed heating of larger particles can cause particle
breakthrough before complete devolatilization, leading to shorter volatile flames, which was measured experimentally and also predicted with CFD. At higher cofiring ratios, the combustion behavior of the wood waste has a larger impact, leading to longer volatile flames and less particle breakthrough.

The impacts of particle breakthrough to the near burner fuel-rich zone can explain the increased N conversion to NO that was shown in previous experimental NO emission measurements. Particle breakthrough couples shorter volatile flame lengths (i.e. shorter fuel-rich regions) with particles devolatilizing in zones of higher oxygen concentrations, which can both lead to increased N conversion to NO. The effects of particle breakthrough were intensified in oxy-fuel flames leading to even higher N conversion to NO.

A simple model was created to predict the presence of particle breakthrough in cofiring flames utilizing gaseous flame and particle devolatilization time scales. A dimensionless number, the Volatile Flame number (VF#), resulted from this work leading to a direct comparison of time scales to determine the critical size for particle breakthrough. All biomass cofired flames were shown to experience particle breakthrough, but the critical size for breakthrough occurs for low cofiring ratios due to the significant particle size difference between coal and wood waste. As the cofiring ratio increases, so does the participation of wood particles in the volatile flame leading to longer flames and less breakthrough. Through this analysis, actions to prevent particle breakthrough including increased turbulent mixing, reduced particle size, and utilization of fuels with high volatile matter contents, were recommended.
8.2 Recommendations for future work

The complexity of the volatile flame zone and its relationship to particle motion and pyrolysis as well as pollutant formation was elucidated in this work. While many research projects focus on solid fuel combustion, the approach taken in this work to understand the flame process is unique. The application of fundamental gaseous flame theories to understand the flame formation processes in pulverized fuel flames has not been completed to the author’s knowledge. This approach has provided the community with a detailed understanding of the behaviors of the volatile flame and the processes occurring within the flame. While, the dimensionless Volatile Flame Number ($VF#$) can be utilized for processes outside of solid fuel combustion and possibly into areas of spray or liquid fuel combustion and advanced combustion technologies of fuel-staging. The following list includes recommendations of future for the continuation of this project:

- Apply the methods and $VF#$ analysis to other fuels. PRB coal is a high volatility coal and wood waste is only one kind of biomass feedstock. Lower volatile coals and different biomass fuels should be fired to see the effects and relationships on the volatile flame length. Other biomass fuels, such as straw or miscanthus energy grasses, can also have more complicated physical features that can lead to more complex interactions.
- Apply this knowledge of the volatile flame and particle breakthrough to changes in fly ash composition, specifically LOI. Similar to the particle sampling done in this work, ash samples can be collected at the end of the flame and downstream. The importance of small versus large amounts of breakthrough on the final ash composition could be determined.
- Complete more oxyfuel combustion measurements and corresponding CFD model results, specifically measuring the volatile flame lengths.
• Complete further validation of the CFD model including temperature and other species measurements for the cases presented as well as for any new cases. Combustor modifications may be required to get more detailed measurements along the length of the combustion chamber. Currently, the discrete measurement ports are located too far apart to capture small-scale changes. More detailed measurements could also provide a means determine the width of the volatile flame region as a function of length in the combustion chamber.

• Further detailed studies into the importance of the partially premixed zone on volatile flame length. These studies would also include impacts to flame stability and particle ignition if applying the VF# analyses.
Appendix A  
Supplementary CFD material

A.1 CFD Methods

Computational fluid dynamics is a set of numerical methods applied to obtain approximate solutions of fluid dynamics and heat transfer problems [157]. CFD utilizes the study of partial differential equations to develop approximate solutions to continuous problems and to questions that cannot be solved analytically. The development of a CFD solution includes the following steps:

- problem statement definition
- CFD type and sub-model selection
- grid construction
- equation and algorithm selection
- boundary and initial conditions
- methods for validation
- assessment of errors and accuracy
- post-processing and visualization of results
- interpretation and analysis of results

While, these are the main steps, the European Research Community on Flow, Turbulence, and Combustion (ERCOFTAC) publishes a best-practices guide [158]. Validation and verification steps are also important ensuring stable, consistent, robust CFD solutions by quantifying solution and code sources of error including [159]:

102
• Insufficient spatial discretization convergence
• Insufficient temporal discretization convergence
• Insufficient convergence of an iterative procedure
• Computer round-off errors
• Computer programming errors

A.2 Conservation equations

For all solutions in ANSYS Fluent, conversation of mass and momentum equations are solved. For the case of pulverized fuel combustion, energy and species conversation equations are also solved. The studies throughout this work focused on two-dimensional solutions with the three-dimensional solutions primarily used for validation and definition of the SO boundary conditions, which will be discussed later. Therefore, the form of the equations discussed will be in reference to two-dimensional axisymmetric solutions, which allow for rotational symmetry around the central axis of the combustion chamber. An x-y plane is constructed and discretized, as shown in Figure 4.1a, which is then rotated around the central axis. This is important to determine which form of the conservation equations are solved.

The following form of the continuity equation is valid for both incompressible and compressible flows in two-dimensional geometries.

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u_x) + \frac{\partial}{\partial r} (\rho u_r) + \frac{\rho v_r}{r} = S_m
\]  

(A.1)
Where $\rho$ is the density of the fluid, $x$ is the axial coordinate, $r$ is the radial coordinate, $v_x$ is the axially velocity component, $v_r$ is the radial velocity component, and $S_m$ is the added mass from the dispersed second phase (e.g. particles).

The following forms of the conversation of momentum equations are given for two-dimensional axisymmetric geometries.

(axial)

$$
\frac{\partial}{\partial t} (\rho v_x) + \frac{1}{r} \frac{\partial}{\partial x} (r \rho v_x v_x) + \frac{1}{r} \frac{\partial}{\partial r} (r \rho v_r v_x) = - \frac{\partial p}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r} \left[ r \mu \left( 2 \frac{\partial v_x}{\partial x} - \frac{2}{3} (\nabla \cdot \vec{v}) \right) \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[ r \mu \left( \frac{\partial v_x}{\partial r} + \frac{\partial v_r}{\partial x} \right) \right] + F_x
$$

(A.2)

(radial)

$$
\frac{\partial}{\partial t} (\rho v_r) + \frac{1}{r} \frac{\partial}{\partial x} (r \rho v_x v_r) + \frac{1}{r} \frac{\partial}{\partial r} (r \rho v_r v_r) = - \frac{\partial p}{\partial r} + \frac{1}{r} \frac{\partial}{\partial x} \left[ r \mu \left( \frac{\partial v_r}{\partial x} + \frac{\partial v_x}{\partial r} \right) \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[ r \mu \left( 2 \frac{\partial v_r}{\partial r} - \frac{2}{3} (\nabla \cdot \vec{v}) \right) \right] - 2 \mu \frac{v_r}{r^2} + \frac{2 \mu}{3r} (\nabla \cdot \vec{v}) + \rho \frac{w^2}{r} + F_r
$$

(A.3)

Where $\mu$ is the dynamic viscosity of the fluid, $w$ is the swirl/tangential velocity component, and

$$
\nabla \cdot \vec{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_r}{\partial r} + \frac{v_r}{r}
$$

(A.4)

### A.3 Conservation equation for swirling flows

An important factor to flame stability in most pulverized fuel systems is a swirling component to the SO velocity. In the laboratory-scale system used in this study (Figure 3.1), two inlets on the
SO are oriented tangentially to the SO axial wall. This design was chosen to provide flexibility in the ratio of swirl to axial velocities in the SO. To solve for the flow field and predict the swirl velocity, the conservation of momentum for the swirl velocity is defined.

(swirl)
\[
\frac{\partial}{\partial t} (\rho w) + \frac{1}{r} \frac{\partial}{\partial x} (r \rho v_x w) + \frac{1}{r} \frac{\partial}{\partial r} (r \rho v_r w) = \frac{1}{r} \frac{\partial}{\partial x} \left[ r \mu \frac{\partial w}{\partial x} \right] + \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^3 \mu \frac{\partial (w)}{\partial r} \right] - \frac{\rho}{r} v_{r,w} \quad (A.5)
\]

A.4 Spatial discretization

This section will discuss the approaches used to apply continuous, integral equations to a discretized computational domain. The equations are dependent upon both spatial and temporal variations. However, all CFD solutions considered in this work are steady-state solutions. The spatial discretization will be discussed, but more about the methods for unsteady solutions and temporal discretization can be found in Pletcher et al. [77].

In the finite-volume method, the scalar transport equations are integrated about each control volume. The conservation equations previously mentioned can be generically described as scalar transport equations. These equations describe the behavior of the dependent variable, or scalar, based on convection, diffusion, and the influence of source terms. The discretized form of the scalar equations are applied to the cells in the computational domain.

\[
\frac{\partial \rho \phi}{\partial t} \bigg|_{time \ derivative} + \sum_{f}^{N_{faces}} \rho_f \bar{V}_f \bar{\phi}_f \cdot \bar{A}_f = \sum_{f}^{N_{faces}} \Gamma_{\phi} \nabla \phi_f \cdot \bar{A}_f + S_{\phi} \bigg|_{source \ term} \quad (A.6)
\]
Where $\phi$ is the scalar quantity (momentum, mass, etc...), $V$ is the cell volume, $N_{faces}$ is the number of faces enclosing the cell, $\rho_f \vec{v}_f \phi_f \cdot \vec{A}_f$ is the mass flux of the scalar quantity through the cell, $\Gamma_\phi$ is the diffusion coefficient, $S_\phi$ is a source term, and $\vec{A}_f$ is the area of the face. The scalar values, $\phi$, are calculated at the cell centers. An upwind differencing scheme interpolates the values from the cell centers to the cell faces to solve the convection terms in Equation 4.6.

The choice of upwind scheme can influence the solution accuracy. In an upwind scheme, the scalar face values are calculated based on cell face values that have been calculated “upwind” or upstream. Many schemes with different formulations and orders of accuracy exist and are discussed in more detail by Pletcher et al. [77]. In this work, a second order upwind scheme, which achieves higher-order accuracy by Taylor series expansion about the cell center, was chosen. To calculate the cell face value, the cell center value from the previous cell is multiplied by a displacement vector.

The diffusion and source terms in Equation A.6 are discretized using a second-order accurate central-difference method. Within the diffusion term is a gradient term to discretize the scalar on the cell face. The gradient term is discretized using the Least Squares Cell-Based Gradient Evaluation method [160]. In this method, the change in the centroid value from cell, $c_0$, to the neighboring cell, $c_i$, that is separated by a distance, $r_i$, can be calculated using the following equation,

\[
(\nabla \phi)_{c_0} \cdot \Delta r_i = (\phi_{c_i} - \phi_{c_0})
\]  

(A.7)

A set of equations can be written for all cells surrounding, $c_0$,

\[
[J](\nabla \phi)_{c_0} = \Delta \phi
\]  

(A.8)
where $[J]$ is the coefficient matrix dependent upon geometry. The coefficient matrix is solved using a least-squares approach by minimizing the sum of the errors associated with each of the equations. Since the coefficient matrix is based on the geometry of the cell center with respect to the neighboring cells, weighting functions, $W_{io}$ are created for each of the cell faces. The gradient is solved by multiply the weighting function by the cell center difference for the $x$, $y$, and $z$ directions. The $x$-direction is shown in Equation A.9. This cell centered scheme is second order accurate.

$$ (\phi_x)_{c0} = \sum_{i=1}^{n} W_{i0}^x \cdot (\phi_{ci} - \phi_{c0}) \quad (A.9) $$

For the second order upwind schemes used for the diffusion term in Equation 4.6, gradient limiters are used to dampen any oscillations that might occur due to sudden changes in the flow field. The standard limiter [161] providing cell to face limiting is utilized in this work. The gradient limiter prevents the variables solved for on the cell faces from surpassing the maximum or minimum values of the neighboring cells. For cell to face limiting, the limited value is restricted to the cell face centers.

**A.5 Segregated solver algorithm**

A segregated, pressure-based solver was chosen to complete the solutions in this work. Figure 4.2 shows the steps taken to solve the momentum and transport equations. In a segregated solver, the momentum and continuity conservation equations are solved sequentially and separate from each other. However, the governing equations are coupled and non-linear, which requires the loop to be solved iteratively to obtain a converged solution. An iterative process to solve the governing equations is needed to ensure conversation of mass and momentum are satisfied. The steps for the SIMPLE algorithm [162], a pressure-velocity coupling algorithm, are broadly defined in Figure 1.
The pressure-velocity coupling requires a pressure correction term because the pressure values are solved at the cell center, while the velocity values are solved at the cell faces. The pressure gradient from one cell center to another across the face acts as a driving force for the velocity behavior at the cell face. To start the solution loop, the first iteration utilizes initial and boundary conditions to provide the first approximations for the momentum equations and the velocity components. The next step is to check the velocity components to ensure that the continuity equation is satisfied. If continuity is not satisfied, then a correction should be applied to the velocity component terms. The velocity terms will have the form of

\[ u_{i+1/2,j} = u_{i+1/2,j}^* + u_{i+1/2,j}' \]  

(A.10)

Where \( u \) is the x-velocity component that is evaluated at the cell face or in between the cell centers in the x-direction, \( u^* \) is the x-velocity evaluated at the previous iteration, and \( u' \) is the velocity component correction term that is used to help satisfy the continuity equation, which is defined by

\[ u_{i+1/2,j}' = \frac{1}{a_{i+1/2,j}} (p_{i,j}' - p_{i+1,j}) \]  

(A.11)

Where \( a_{i+1/2,j} \) is a multiplier term that is dependent upon grid spacing and also neighboring velocity terms. The \( p' \) terms are pressure correction terms. The next step is to apply the updated velocity component terms to the continuity equation and solve for \( p' \). This completes one iteration of the pressure-correction equation step and the new velocity components can be used to solve the remaining transport equations. Iterations of this process will continue until convergence is reached.
A.6 Turbulence Model Specifications

The Reynolds form of the momentum equations is

$$\frac{\partial}{\partial t} (\rho \bar{u}_i) + \frac{\partial}{\partial x_j} (\rho \bar{u}_i \bar{u}_j) = -\frac{\partial \rho}{\partial x_j} + \frac{\partial}{\partial x_j} (\overline{r_{ij} - \rho \bar{u}_i \bar{u}_j}) \quad \text{(A.12)}$$

where \(\bar{u}\) components are time-averaged components and \(\overline{r_{ij}}\) is defined by

$$\overline{r_{ij}} = \mu \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \quad \text{(A.13)}$$
The averaged fluctuating velocity term, \( \bar{u}_i \bar{u}_j \), are apparent stresses known as Reynolds Stresses, which are modeled in the RANS approach using the Boussinesq approach [163]. The Reynolds stresses are related to mean velocity gradients utilizing a turbulent viscosity \( \mu_t \), turbulence kinetic energy \( k \), turbulence dissipation rate \( \epsilon \), or specific dissipation rate \( \omega \) as follows

\[
- \rho \bar{u}_i \bar{u}_j = \mu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \left( \rho k + \mu_t \frac{\partial u_k}{\partial x_k} \right) \delta_{ij}
\]  

(A.14)

The turbulent viscosity is related to the turbulence kinetic energy through the following relations

(Turbulence Kinetic Energy)

\[
\frac{\partial k}{\partial t} + U_j \frac{\partial k}{\partial x_j} = P_k - \beta^* k \omega + \frac{\partial}{\partial x_j} \left[ \left( \mu + \sigma_k \mu_t \right) \frac{\partial k}{\partial x_j} \right]
\]  

(A.15)

(Specific Dissipation Rate)

\[
\frac{\partial \omega}{\partial t} + U_j \frac{\partial \omega}{\partial x_j} = \alpha S^2 - \beta \omega^2 + \frac{\partial}{\partial x_j} \left[ \left( \mu + \sigma_\omega \mu_t \right) \frac{\partial \omega}{\partial x_j} \right] + 2 \left( 1 - F_\omega \right) \sigma_\omega \omega \frac{1}{\omega} \frac{\partial k}{\partial x_i} \frac{\partial \omega}{\partial x_i}
\]  

(A.16)

The variables not previously defined in Equations 4.15 and 4.16 are closure coefficients and constants specific to the SST \( k - \omega \) model and can be referenced in Menter, [82]. The \( k - \omega \) formulation is usable in boundary layers and can be used as a Low-Re turbulence model without any extra damping functions, such as the formulations used in the \( k - \epsilon \) models. For the free stream flow, the SST formulation switches to \( k - \epsilon \) formulation.
A.7 Discrete Phase Model

The equations of particle motion include a force balance around the particle. Drag, gravity, virtual mass, and pressure gradient forces are included.

\[
\frac{du_p}{dt} = F_D(u - u_p) + \frac{g_x(\rho_p - \rho)}{\rho_p} + F_x
\]  

(A.17)

Where \(u_p\) is the velocity of the particle, \(F_D\) is the particle drag force, which is a function of the Reynolds number and drag coefficient, \(u\) is the time-averaged mean velocity of the homogeneous phase, \(g_x\) is the velocity force, and \(F_x\) represents the addition of remaining forces not listed in this equation.
Appendix B
30 kWth solid fuel combustor standard operating procedure (SOP)

B.1. Coal/Biomass furnace emergency shutdown procedures

1) STOP coal feeder and/or close the FUEL valve (if running propane).
2) Close SO CO₂ and SO O₂ valves. Keep SO AIR running or else introduce some SO AIR
3) Turn off SHAKER AIR (if running coal).
4) Reduce pressure and close the valves for PRIMARY-1 and PRIMARY-2 gases.
5) Turn the SO MIX pressure and flow down low in order to keep some air moving through the system to ensure the refractory does not cool too quickly.
6) Bleed the PROPANE line by closing the tank and keeping the air flows inside the system at settings you used during your experiment before shutting off the gas supply on the flow panel.
7) Close PROPANE valves in the central line on the ceiling hang down island.

B.2. Pulverized fuel system operating procedure

B.2.1 Preliminaries

1) Check calibration of CEM and recalibrate if needed.
2) Fill coal and sawdust hoppers.
3) Please wear flame retardant lab coat and safety glasses
B.2.2 Ignition

1) Verify that all valves on panel, ignition wand valve, regulators, and flow meters are closed except for SO Mix Swirl (valve should be wide open).

2) Open SO AIR valve and set secondary air to 50 psig and just crack valve until SO MIX SWIRL to 3 SCFM.

3) Open PRIMARY-1 air valve and set primary air to 50 psig and set the tube cube scale reading to 20 for steel ball.

4) Open PRIMARY-2 valve and set tube cube using the steel ball to adjust the pressure at the eductor cap to 0.2 inH2O reading from the magnahelic mounted next to the feeders. KEEP AN EYE ON THE PO CAP PRESSURE EVERY TIME THE FLOWS ARE ADJUSTED.

5) (Ignition wand operation needs 2 people: one person at the flow panel and the other operating the ignition wand) Open propane tank and set tank regulator to ~40 psig. (NOTE: IT IS CRITICAL THAT THE PILOT FLOW METER VALVE IS CLOSED TO PREVENT THE BUILD UP OF A POTENTIALLY DANGEROUS PREMIXTURE IN THE COMBUSTOR)

6) Set fuel regulator on flow panel to <5 psig.

7) Turn the valve on the ignition wand very slightly open, light ignition wand.

8) Slowly increase gas pressure on flow panel fuel regulator, while decreasing gas flow on ignition wand, until gas pressure is 25 psig, and flame is of desired size.

9) Check to make sure gas flowrates inside the furnace will not put out the flame by holding the wand close to the ignition port. If gases are blowing out, then check the pressure in the filter bag or reduce flows. The system should be close to atmospheric pressure when trying to insert the wand. Insert into ignition port. Verify visually that ignition wand remained ignited and centered in the combustion chamber.
10) Open pilot gas flow meter valve and set steel ball scale to 10 to ignite pilot flame. Check for pilot flame. (If pilot flame is out, stop propane supply at flow panel shut off valve, flush system with air for 2 minutes. Then begin again at Step 5)

11) Increase SO MIX SWIRL to 5.8 SCFM and set the PO CAP to maintain 0.2 inH2O.

**B.2.3 Increase thermal input**

1) **TWO PERSON JOB:** ONE PERSON INCREASING FLOWS AND THE OTHER WATCHING THE FLAME. Increase fuel, and PO air incrementally until PO air is at 45 steel ball, and Fuel is at 145 steel ball (on 603D rotameter) (28 on steel ball when using 604B rotameter). Fuel flow should be incremented in steps of 10 on the steel ball. PRIMARY-1 flow should be incremented in steps of 5 on the steel ball. Observe flame after each step change. If flame starts to fluctuate, usually can be corrected by increasing PO air. If flame appears dark, or sooty, PO air should be increased.

2) Set SO AIR to 6.5 SCFM @ 50 psig, SO MIX SWIRL to 7.3 SCFM, SO MIX AXIAL to 5.5 SCFM and the PO CAP to maintain 0.2 inH2O.

3) Remove pilot wand after stable flame conditions are attained.

**B.2.4 Coal delivery (Work in progress with new burner)**

1) Connect Horiba to exhaust to measure O2 and CO. Make sure oxygen matches spreadsheet predicted value and CO is close to zero.

2) Turn on SHAKER AIR to 40 psig.

3) Set SO AIR to 6.5. Set the PO CAP to maintain 0.2 inH2O.

4) Set SO MIX SWIRL to 9 and SO MIX AXIAL to 3.

5) Increase PO air to 50 on steel ball and set the PO CAP to maintain 0.2 inH2O.

6) Decrease PROPANE fuel to 85 (on 603D rotameter) on steel ball.
7) Turn on coal at 180 RPM and set the PO CAP to maintain 0.2 inH2O.

8) Turn down PROPANE fuel to 35 (on 603D rotameter) and check for stable coal flame. If stable, then turn propane fuel off.

B.2.5 Running oxyfuel conditions with recycled flue gas (RFG)

**UNDER CONSTRUCTION**

B.2.6 Shutdown

1) STOP coal feeder and turn off SHAKER AIR

2) Turn off PRIMARY-1 AND PRIMARY-2.

3) Turn the SO MIX pressure and flow down low in order to keep some air moving through the system to ensure the refractory does not cool too quickly.

4) Bleed the PROPANE line by closing the tank and keeping the air flows inside the system at settings you used during your experiment before shutting off the gas supply on the flow panel.

5) Close PROPANE valves in the central line on the ceiling hang down.

6) Close all SO and PO valves.
Appendix C
Considerations for decision-making on distributed generation in rural areas

**This paper has been submitted to Energy Policy and is currently under review.**

Melissa L. Holtmeyer*, Shuxiao Wangb, Richard L. Axelbaum*

*a Department of Energy, Environmental, and Chemical Engineering
Washington University in St. Louis, St. Louis, MO 63130

b Department of Environmental Science and Engineering
Tsinghua University, Beijing, 100084, China

C.1 Abstract

Energy resources for rural electrification are variable and widely dispersed such that a solution for one region might not be appropriate for another. This study evaluates the feasibility of coal-fired and renewable technologies for distributed generation in areas that are either isolated from the centralized grid or are striving for greater independence from the grid. The renewable power generation options considered are solar photovoltaic and wind power, with battery storage or fossil fuel generator backup. New local coal-fired power, as well as extension of the grid from the existing centralized power system, are considered to compare the impacts of scale and traditional approaches to power generation. A multi-criteria approach, which includes technical, economic, social, and environmental variables, is described for a case study in rural northwestern China to demonstrate the complexity of energy decision-making. Economic factors, including cost of electricity generation, breakeven grid extension distance, capacity
shortage fraction (the ratio of the annual capacity shortage to the annual electric load) and land use are evaluated.

C.2 Keywords

Distributed generation; Renewable energy; Multi-criteria approach

C.3 Introduction

Approximately 1.5 billion people worldwide lack access to electricity, 84% of whom live in rural areas of developing countries [164]. China, like many developing countries, is paving the way for industrialization by building centralized grids to electrify major population centers. However, this approach to electrification is not always amenable to rural areas, especially in remote areas. Extension of the centralized grid to remote or underdeveloped areas is often not practical due to geographic isolation, limited electricity demand or economic constraints. Furthermore, installation of a new grid can be slow, and even if one exists, load shedding can result in unreliable power for lower-priority regions on the grid.

Distributed generation (DG) systems, ranging from a few kilowatts to tens of megawatts, produce power locally with the goal of only providing for the nearby populous. Grid losses, which are intrinsic to centralized power generation, are minimized since the DG system is typically located near the demand. DG systems can also provide economic and political benefits through local control in off-grid or grid-connected options. When a reliable supply of energy resources is located near the service area, off-grid DG can produce reliable power that is independent of the grid and has reduced environmental impacts [165]. Distributed generation systems can also be connected to the grid with options to sell power to the utilities during times...
of surplus. However, the primary function of the grid-connected DG system is to provide power to the local community.

In the past when establishing the power infrastructure, industrialized countries relied on fossil fuels, primarily coal, to bring reliable power to manufacturing and population centers. With the threat of resource constraints and climate change, industrialized countries have since begun implementing renewable energy in a grid-connected manner. Developing countries, on the other hand, can approach industrialization with a mixed portfolio of energy options, often without the established fossil-fuel infrastructure, particularly the centralized grid. Diverse energy portfolios with both renewable and fossil fuel technologies can also help meet regulations on energy and environment.

Renewable DG has been considered not only to increase generation capacity, but also to electrify regions that are otherwise unreachable [166–169]. Wind, mini-hydro, and wood-fired grid-connected DG power plants in Sri Lanka have reported reduced emissions with only marginal cost-increases compared to large hydropower and coal-fired power plants due to reductions in transmission and distribution losses [170]. Bangladesh, which also has abundant renewable resources, has considered DG to provide power for the 70% of the population that presently does not have access to electricity [171]. Renewable energy sources can be more naturally utilized in a distributed generation manner, by meeting the energy demands of the population in the vicinity of the plant, but as local economies expand and industrialize, the electricity demands increase, as does the need for highly reliable power.

Coal power plants can provide low-cost and reliable electricity. For this reason they are heavily utilized in countries like China, India and the U.S. that have abundant coal reserves and large demand. Coal-generated electricity has a significant economic advantage over wind and solar at
large scale, but at smaller scales, the cost of electricity generation from coal increases and the complexity of the power plant can tax the skills of the local community. Therefore, a balance of large-scale and distributed generation of both fossil fuel and renewable energy should be considered to optimize the utilization of resources and minimize costs and environmental impact.

Selection of appropriate generation technologies is largely based on techno-economic analyses. However, decision-making for DG should include both financial and non-financial factors when identifying appropriate technologies. Multi-criteria decision-making methodologies provide ways to evaluate the viability of technologies when considering technical, economic, environmental, and social variables [172]. This approach allows for the comparison of different technologies or the assessment of a single technology, independent of scale and location [173–175]. By considering many criteria, the decision-maker can focus on opportunities and constraints, allowing the most desirable technologies to be identified [176].

This study takes a multi-criteria decision analysis approach to evaluating the appropriate scale and technology of DG for a case study in rural China. Technical, economic, environmental, and social factors are used to compare small- and large-scale renewable and non-renewable power generation technologies. The importance of renewable resource availability is also addressed. Wind and solar photovoltaic (PV) power with battery or diesel generator backup are compared with coal-fired power to understand the fundamental issues associated with DG and how they are influenced by scale.
C.4 Considerations for technology viability

For rural areas that have adapted to a lifestyle with either unreliable or infrequent access to power, the addition of a DG system can greatly improve quality of life. The ability to complete one’s work or studies at night can enhance both the social and economic status of a community. However, the decision to update power systems and/or to build new power plants is complex with many variables that are interconnected. For DG power systems, a demand-side matching of current and future energy needs with the capabilities of the power plant is the best way to ensure the success of the project.

The casual loop diagram in Figure 1 was created with the goal of understanding how social variables, which include the needs of the community, can impact choices of technology. This diagram also conceptualizes the complex relationships between technical, economic, environmental, and social variables, which are included in power generation decision-making to ensure community acceptance and long-term sustainability. Major social drivers (variables located in the inside box) influence decisions of technology based on the direct connections to power generation variables (outside box).
During the planning stages, a balance between economic and social effectiveness can cause certain technologies to be favored over others. Small-scale projects are perceived to have lower negative impacts on the local community and natural environment, but the cost per unit output of these projects is typically higher than that of large-scale technologies [175]. Further trade-offs between scale, resource availability, and environmental impacts will be identified for a case study in rural China.

C.5  Power generation in rural China

Over the past 20 years, China has reached a 98% electricity access rate for all major cities and has connected an additional 900 million rural residents to provincial and national grids [177].
However, an estimated 100 million rural people still have insufficient power or lack access to a power source [178]. One of the regions of large power deficiency in the country is in Xinjiang province, where approximately 17% of the population is without access to electricity [179]. Distributed generation projects have the potential to greatly impact the local economy and livelihoods of people in this area. However, the choice of DG technology can vary greatly from region to region, and an all-encompassing technology does not exist.

C.5.1 Case study for Xinjiang province, China

The northwest region of China is home to 30% of the country’s coal reserves, which is expected to drive a shift in the coal production base from the east coast to the north and northwest [173]. Xinjiang has also become the largest producer of oil and natural gas in the country. Consequently, power capacity expansion will be needed throughout the province if a shift in population occurs due to the economic opportunities afforded by these vast resources. The fossil fuel resources are currently being prioritized for the east coast where the major population and manufacturing centers are located [181].

This study will focus on power generation options for Burqin County, Altay Prefecture, Xinjiang Province, where one of the authors, MLH, visited to assess the current energy situation and needs. Discussions with local community members and leaders formulated the community input. Burqin County is a rural community with people living and working in the central city and also along the outskirts as semi-permanently settled nomadic herders. A large percentage of the population works in the farming and animal husbandry industries. Burqin County is located at a latitude of 47°50’N and a longitude of 88°8’E, has an annual average wind speed of 4.5 m/s and an average solar radiation of 4.5 kWh/m²/day. The population of 67,700 lives in 19,500 households [182] with an average household electricity demand of 586 kWh/year [183].
and a current peak demand of 3 MW. The peak demand times are in the early morning and early evening before sunset. The current cost of electricity for the residents of Xinjiang is approximately $0.06/kWh [184], which is potentially subsidized by the Chinese government [185].

Burqin County is located 686 km north of the capital city, Urumqi, where the provincial grid is centered. Unless the provincial grid is expanded beyond its current boundaries, there will be significant portions of the province that will not be connected to the grid. Thus, new DG technologies could be valuable to these communities. The primary methods of power generation around Burqin County are small-scale coal-fired power plants and hydropower connected to a local grid. The semi-nomadic herders have access to portable individual household-sized (~10 kW) solar PV and hybrid solar PV/wind systems that are used to power small electronics and lights. These have been made accessible through funding from non-governmental organizations (NGOs) and the local government. They are not allowed to connect to the local grid. Consideration of DG systems would allow Burqin County to increase electricity capacity and to include the herders’ energy needs, while utilizing low emission and/or renewable energy.

C.6 Methods for economic analysis

The financial analysis was performed using the National Renewable Energy Laboratory’s Hybrid Optimization Model for Electric Renewables (HOMER) for renewable energy technologies and the National Energy Technology Laboratory’s Integrated Environmental Control Module (IECM) for coal power plants.
C.6.1 HOMER: Hybrid Optimization Model for Electric Renewables

With HOMER, renewable and distributed micro power systems can be designed and compared using information about local conditions, resource availability and electricity demand profiles. For this study, only off-grid solar PV and wind DG technologies are considered. The power systems include equipment to generate electricity (PV panels or wind turbines), and convert (converters or inverters) and store (batteries) the electricity. Another option considered for the renewable energy systems is a fossil-fuel backup generator instead of battery storage. Financial and technical feasibility are incorporated using optimization and sensitivity analysis algorithms to determine the best power generation option based on cost and resource availability [186]. HOMER simulates probable combinations of power systems, and then ranks them based on their net present costs. These costs include expenditures incurred over the lifetime of the project, including capital costs, operation and maintenance, and replacement.

Inputs for the wind and solar resources include monthly averages with advanced parameters, as shown in Table 1 for the wind speed distribution, which characterize the small variations in the resource availability.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Anemometer height (m)</td>
<td>60</td>
</tr>
<tr>
<td>Weibull k</td>
<td>2.1</td>
</tr>
<tr>
<td>Autocorrelation factor</td>
<td>0.8</td>
</tr>
<tr>
<td>Diurnal pattern strength</td>
<td>0.09</td>
</tr>
<tr>
<td>Hour of peak wind speed</td>
<td>16</td>
</tr>
</tbody>
</table>

The solar global horizontal radiation and the clearness index (fraction of the solar radiation that is transmitted through the atmosphere to strike the surface of the Earth [186] were calculated
from the HOMER database based on the latitude and longitude of Burqin County. The best possible resources were calculated in the same manner.

For the wind power analyses, the Vestas V52-850 wind turbine was assumed. The peak power output of the wind turbine is 850 kW and the rotor diameter is 52 meters. The installed cost of this wind turbine was assumed to be $167,000.

HOMER assumes solar panels are equipped with a maximum power point tracking (MMPT) converter, which maintains a linear relationship between the power output of the solar array and the incident solar radiation. This type of converter ensures that the maximum power available from the cell or array is extracted. The solar panels were assumed to have a 20% efficiency, fixed location with optimal alignment with the sun’s direction, and were estimated to cost $6/Wp installed, which includes replacement and operations and maintenance costs [187]. While the prices for solar panels continue to drop, this price and efficiency represent upper bounds. The choice of wind turbine and solar PV panel were held constant throughout this study.

For energy storage and backup power options, deep-cycle renewable energy batteries [186] and diesel fuel generators were considered. The diesel generators were first sized to match the peak load, and then followed by an optimization in HOMER to calculate the number of wind turbines or solar panels. The price for diesel fuel was assumed to be $1.01/L [188].

One component of the economic analysis is a comparison of the impacts of resource availability. Comparisons will be made between Burqin County conditions and best possible conditions. The best possible conditions are those of places from around the world that have the best resource availability on land. The best possible annual average wind speed of 8.12 m/s is assumed [189].
The best possible annual average solar radiation of 6.156 kWh/m$^2$/day is assumed [186]. Comparing the results in Burqin County with the best possible conditions allows for an understanding of how local conditions are affecting the economics and allows for an upper bound in the potential for the renewable resources.

### C.6.2 IECM: Integrated Environmental Control Module

Performance and cost estimates for conventional coal-fired power plants were obtained with IECM. IECM includes a systematic analysis of emission control options, including pre-combustion, combustion and post-combustion methods [190]. For this study, the costs for a supercritical pulverized coal power plant with emissions control for SOx, NOx, PM, and Hg were evaluated. The limits for SOx, NOx, and PM emission are based on the current U.S. New Source Performance Standards. Currently there are no power plant Hg standards for emission limits, but 95% removal for oxidized Hg and 39% removal for elemental Hg were assumed. By considering best possible emissions control for coal, the comparison between renewables and coal is made with both forms of power generation having minimal local environmental impact.

Pollution abatement technologies selected for this study included a pulse-jet fabric filter for particulate control, low-NOx burners with overfire air for NOx control, wet flue gas desulfurization (FGD) for sulfur control, and activated carbon injection for mercury control. A medium sulfur bituminous coal with a delivered cost of $3.420/MBtu [191], which includes transportation costs to rural areas, was assumed. The costs of the power plant equipment were based on default values in IECM, but with labor costs assumed for rural areas in China [192].

Carbon capture and storage (CCS), which is considered to be an important component of large scale coal-fired power generation in the future [193] is not considered in this study because
political and economic uncertainties exist with respect to its implementing. The cost of implementing CCS is estimated to increase the costs of electricity from coal by 50-100%.

C.7 Cost of electricity generation from renewable technologies

Burqin County is a combination of rural and remote-rural areas in northwestern China where the demand for electricity is growing, as is the concern for the environment. As noted, renewable energy technologies, which are most commonly installed as distributed generation systems, can increase the local community’s access to electricity. This analysis is focused on the viability of off-grid DG systems. An economic comparison between Burqin County and best possible scenarios demonstrates the challenges and opportunities with using renewable energy technologies. The costs of electricity generation are assessed using variables that are closely related to the social and environmental aspects, including capacity shortage fraction, land usage, and breakeven grid extension distance.

Electricity demand in underdeveloped areas differs significantly from that of developed areas, where reliability of the electricity supply is crucial to support the economy. In developing countries or rural areas like Burqin County, the reliability of the supply can be less stringent and thus traditional forms of electrification are not necessarily required. The capacity shortage fraction, which is the ratio of the annual capacity shortage to the annual electric load, captures the fraction of the electric load demands that are not being met. Figure 2 shows the relationship between the costs of electricity generation and the capacity shortage fraction for best possible and Burqin County conditions of wind and solar PV at a peak demand of 5 MW.
The cost of generation in Figure 2 has been optimized with the amount of battery storage, PV panel or wind turbine capacity, and converter size for a specific capacity shortage. Increases in battery storage and PV panels and/or wind turbines are required to provide consistent power for small capacity shortage fractions, leading to a sharp increase in the costs of generation as the capacity shortage approaches zero. The cost of wind power generation is always less than that of solar. The cost of generation for solar PV would not be affordable for the people of Burqin County even if the solar resources where ideal. The cost of generation for wind power in Burqin County is also too expensive, particularly at low capacity shortages, but if the population can accept higher capacity shortages, then the costs are similar to the current price for electricity.

**C.7.1 Impacts of Resource Availability on Costs of Generation**

While it is valuable to understand the optimum cases for wind and solar by assuming the *best possible* conditions, most areas, including Burqin County, do not possess ideal resources. Figure 3 shows the cost of electricity generation for wind power as a function of the capacity shortage fraction for four different wind speeds.
When analyzing Figure 3, it is important to take into consideration the operation of the wind turbine. The cut-in speed for the Vestas V52-850 is 4 m/s and the cut-out speed is 25 m/s [194]. The power curve rapidly increases for wind speeds above 5 m/s and plateaus at 15 m/s, where the wind turbine will regulate the rotors in order to prevent stalling. The cost of generation decreases rapidly as wind speed increases past the cut-in speed. Even though the power gain between 8.12 and 16 m/s is greater than the gains between 4 and 8.12 m/s, the reductions in generation costs are small. The electricity costs are determined based on the electricity delivered to the load, not the electricity produced. At the times when the wind speeds are high enough to produce more power than what is needed, excess power is produced that cannot be used or stored. The issues of intermittent and hard to predict resources will be discussed in the following section.

The impact of resource availability on the cost of electricity generation can be best seen when comparing the best possible conditions to the conditions of Burqin County, which has an
average wind speed around 4 m/s. For the majority of the capacity shortage fractions, the cost of electricity generation is approximately four times the cost under best possible conditions. Similar trends can be seen for solar PV power (not shown) when the average solar radiation or the clearness index are less than ideal. For Burqin County, the cost of electricity generation from a 5 MW DG system is much higher than current prices; therefore, even for high capacity shortage fractions significant subsidies would be needed.

C.7.2 The intermittency of renewable resources

While capacity shortage identifies the yearly mismatch between supply and demand, instantaneous data reveals diurnal shortfalls in supply. To illustrate this, the line plots shown in Figures 4a and 4b show the instantaneous mismatch between electricity supply from wind and a typical demand curve for a week in Burqin County. This example is for a 20% capacity shortage and an annual average wind speed of 4 m/s calculated from HOMER. Figure 4a shows the hourly data during a week for the primary (electricity) load and the power generated from the wind turbines. Times of high and low wind turbine power production exist where the turbines are producing either excess electricity or not enough. Figure 4b illustrates the times of excess production and unmet demands, which directly correspond to the primary load and wind turbine production curves in Figure 4a. On the evening of January 23, for example, the primary electricity demands could not be met, as shown by the peak in the unmet load curve. Power production is too low, as shown in Figure 4a, and the stored battery power has been drained, as indicated by the rapid decrease in the battery state of charge. Conversely, on January 24, power production is very high during the day, exceeding the primary demands and allowing for recharging of the batteries. The amount of battery storage, which has been optimized to minimize cost of electricity, cannot store all of the excess energy, nor can it provide all the energy needed when there is no wind. Doing so would dramatically increase costs.
If technologies are not properly designed with regards to resource intermittency, then the community would experience excessive capacity shortage, leading to an increase in the frequency of times and duration throughout the year when demands are not met. Despite these constraints, the addition of new renewable DG systems can increase the overall availability of power in the area with reduced environmental impacts.

C.7.3 Low Capacity Shortage Fractions with Diesel Generator Backups

Historically, stand-alone small-scale diesel or gasoline generators, or renewable energy systems combined with backup generators, have provided more reliable power for small-scale demands when the centralized grid cannot be extended [195]. These systems can provide low capacity shortage fractions, but can be expensive and have negative environmental impacts. Also, volatile fuel pricing and uncertainties associated with fuel availability and equipment maintenance can lead to uncertainties in costs and reliability.
Table 2 compares the cost of generation using a backup diesel generator with that of battery storage for wind and solar PV systems under *best possible* conditions for a 5MW rated capacity. The diesel generator backup is assumed to have a capacity shortage of less than 0.1%, which assumes minimal down time due to equipment failures and maintenance. While the capacity shortage is low with the diesel backup, the cost of generation from wind power can be significantly higher than it is with battery backup with a larger capacity shortage e.g., there is a 63% higher cost for 5% capacity shortage and 333% higher cost for 40%. However, the costs are similar for solar PV with diesel back-up and battery back-up with 5% capacity shortage. For this scenario, trade-offs would have to be made between the variability and availability of fuel versus the sun’s intermittency. For a 40% capacity shortage, diesel back-up is 28% more expensive.

### Table 2. Cost of generation for 5 MW peak demand with *best possible* resources.

<table>
<thead>
<tr>
<th>Generation System</th>
<th>Capacity Shortage (%)</th>
<th>Cost of Generation ($/kWh)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wind with Generator</td>
<td>&lt;0.1</td>
<td>0.26</td>
</tr>
<tr>
<td>Wind with Batteries</td>
<td>5</td>
<td>0.16</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>0.06</td>
</tr>
<tr>
<td>PV with Generator</td>
<td>&lt;0.1</td>
<td>0.51</td>
</tr>
<tr>
<td>PV with Batteries</td>
<td>5</td>
<td>0.54</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>0.4</td>
</tr>
</tbody>
</table>

The backup generator was used 68% of the time for PV and 14% for wind power. For solar PV systems, the generator usually runs throughout the night and at times of the day when sufficient sun is not available. On the other hand, excess electricity is produced because the backup generator does not provide any storage. Wind power produced 63% excess, while PV power produced 29% excess.
C.7.4 Land Use Requirements for Renewable Energy Technologies

The amount of land required for power generation equipment is directly related to the capacity shortage, as shown in Figure 5 for best possible and Burqin conditions. The land required is for power generation equipment only, and does not include that for battery storage, backup generators or maintenance. The sharp increase in land use as the capacity shortage fraction goes to zero for wind power is derived from the significant addition of wind turbines to generate increased power during times of low wind speeds. The methods of [196], which account for the distance between turbines to reduce interference of the wake of the turbine blades, was used to calculate the land requirement for wind turbine installations.

![Figure 5. Land use requirement as a function of capacity shortage for 5 MW peak demand.](image)

Solar PV panels can be placed very close to each other without interference, thus reducing the overall land required. However, unlike wind turbines, solar panels completely cover the land and do not allow for growth of vegetation. A linear trend exists for PV when only the land required for the panels is included. Wind turbines can have a more modest impact on land when
the space in between the turbines is utilized for other purposes. The land necessary for battery storage is dependent upon demand and the capacity shortage fraction, but is negligible compared to the land needed for generation.

For low capacity shortages with battery backup, land use requirements and the cost of generation have a complex relationship. Wind power has a lower cost of generation with significant land use, while PV power has a high cost of generation with reduced land use. These trade-offs can be important for the people of Burqin County who rely on the land for their livelihoods and who cannot afford high costs for energy. The amount of land that wind turbines would occupy significantly increases for wind speeds in Burqin.

### C.7.5 Options for Centralized Grid Extension

In regions with less than ideal resources, system requirements for renewable DG can become more expensive, less reliable, and more land intensive. Another option for improving access to electricity in regions like Burqin County is to extend the local grid to the centralized grid. The breakeven grid extension distance, which is the minimum distance from the grid where a stand-alone system is less expensive than extending the grid, can be used to determine the viability of extension and connection to the centralized grid. For negative breakeven grid extension distances, the renewable DG technology is always favored over extension of the centralized grid. The lines in Figure 6 represent the breakeven grid extension distances for wind and solar PV, considering both Burqin County and best possible resource conditions. For this comparison, a 40% capacity shortage is assumed. The cost of transmission lines was assumed to be the average capital cost for 220 kV transmission lines in China in 2007 of $40,947/km [182].
Figure 6. Breakeven grid extension distance for wind and solar power systems with 40% capacity shortage for different resources.

Figure 6 demonstrates the sensitivity of DG systems to resource availability and scale. Wind power systems are always favored over centralized grid extension for best possible conditions. The wind power breakeven distance for a 5 MW peak demand in Burqin County is 60 km and the distance to the province's centralized grid is 686 km. Therefore, implementation of a new DG system would be recommended over grid extension. The breakeven grid extension distance for PV power in Burqin is 566 km. Thus, PV power would also be recommended over extending the centralized grid.

C.8 Coal-fired power generation

China and India have large coal reserves, rapidly developing economies, and millions of people in rural communities lacking access to steady electricity, therefore, coal-fired power is also an option. Coal-fired technologies follow the economies of scale and are more expensive at small-
scale due to the substantial costs of capital equipment and labor. There are many operational issues with new coal-fired power that will not be addressed in this study, but by including coal in this analysis, a comparison can be made between the costs and scale of coal-fired power to renewable energy systems. As a point of reference the cost of generation is first calculated assuming no emission controls. At ~0% capacity shortage the cost of generation ranges from $0.097/kWh for 100 MW systems down to $0.075/kWh for 900 MW systems. For this analysis, coal-fired power plants below 100 MW were not considered due to limitations in IECM.

Coal-fired plants must meet varying regulations on emissions, depending on the policy of the local government. Figure 7 shows the approximate incremental cost increases for emission controls for PM, NOx, SOx, and Hg. Sulfur control by FGD contributes over half of the cost increase for the range of power plants considered. The ability to utilize low sulfur coal could eliminate this cost, but could also add to the fuel costs. Adding all of the emission control equipment to a 100 MW system adds approximately 20% to the cost of electricity generation over the base plant. Note that this relatively small increase in the cost of generation is due to the smaller plant size and the high cost of coal.

![Figure 7. Increases in the cost of electricity with various emission controls for coal-fired power systems.](image)
The cost of generation for a 100 MW coal-fired power plant with all emissions controls is $0.123/kWh. This is the smallest and most expensive plant considered, and, as seen from Figure 7, the increases in the cost of electricity generation decrease and eventually plateau as plant size increases due to the economies of scale. A 5 MW wind power system with best possible conditions and a 10% capacity shortage has a similar cost of generation to the 100 MW coal plant. While the cost to generate electricity is similar, the scale, infrastructure requirements, and land use of the systems is significantly different. For the average wind speed and solar radiation of Burqin county renewable power is always more expensive than a 100 MW coal-fired power plant, as can be seen from the cost of generation in Figure 2. This conclusion assumes coal resources and infrastructure are available or can be made available. Coal is also particularly attractive when a low capacity shortage and a large electricity demand are required, for example, where there is a manufacturing base in the service area. In contrast, renewable DG is particularly favorable for smaller demands and areas accepting of higher capacity shortages and the desire to reduce environmental impacts. The demands of Burqin County are not sufficiently high to support even a small scale coal-fired power plant. However, as future demands grow and industries develop, coal-fired power may become a viable option for this region.

C.9 Conclusions

Renewable distributed generation was evaluated as an alternative to traditional centralized power in rural areas where the electricity demand differs significantly from that of developed areas. In developing countries or rural areas like Burqin County, the reliability of the supply can be less strict leading to the inclusion of non-traditional forms of electrification. Renewable energy technologies are best utilized at smaller scales in a distributed type manner, whereas coal-fired technologies employ the economies of scale and are best utilized at much larger scales.
The application of renewable energy at larger scale (~500 MW) or coal-fired power at small scale (~10 MW) is not feasible due to the technical, social, environmental and political factors that were discussed in this study.

Renewable DG projects can provide opportunities to generate electricity for local consumption with low environmental and societal costs, if the many factors included in this study are considered. The availability of wind and solar resources is location dependent and intermittent, which impacts the cost of generation and land use requirements. For areas with non-ideal conditions, low capacity shortages and/or higher power outputs could become very costly. However, coal-fired power can provide a reliable electricity supply for expanding areas or manufacturing bases, but with environmental and social costs depending on pollution abatement equipment investments and the conditions of the current infrastructure. The technical factors coupled with social factors (i.e. the current and future needs of the community), can be major drivers towards the final technology choice, and ultimately public acceptance.

**C.10 Acknowledgement**

This work was funded in part by a grant from the McDonnell Academy Global Energy and Environment Partnership (MAGEEP) at Washington University in St. Louis in collaboration with Tsinghua University. M.L.H was supported in part by a U.S. EPA STAR Fellowship. The authors would like to thank Mr. Will Slater for his assistance with the cost analysis and Mr. Daniel Conner for helpful discussions with respect to the causal loop diagram presented in the case study.
References

[80] Imperial College London, (2012).
Curriculum Vitae

Melissa Holtmeyer

holtmeyerm@seas.wustl.edu

Summary

Fall 2012 Ph.D. graduate in Energy, Environmental & Chemical Engineering seeks a research position to continue the pursuit of high quality, collaborative research in the areas of advanced combustion, computational fluid dynamics (CFD), alternative fuel technologies, and energy policy. Proven leadership, communication, and design skills; collaboration and organizational strengths.

Education

Washington University in St. Louis, St. Louis, Missouri

Ph.D. Energy, Environmental, & Chemical Engineering 2012
Advisor: Dr. Richard Axelbaum
Dissertation title: The impact of biomass fuels on flame structure and pollutant formation during biomass cofiring combustion
GPA: 3.96

M.S. Mechanical Engineering 2007
Specialization: Fluid Thermal Sciences
GPA: 3.83

B.S. Mechanical Engineering, magna cum laude 2006
GPA: 3.79

Research Interests & Experience

U.S. EPA Science to Achieve Results (STAR) Fellow 2010 - Present
Washington University in St. Louis
Project: Clean Energy Research and Education
Fundamental combustion research and interdisciplinary energy and environment course development provide a well-rounded understanding of the challenges with our future’s energy portfolio.
- Research: The impacts of biomass fuels on volatile flame length and pollutant formation during biomass cofiring combustion using both experimental methods and computational fluid dynamic modeling
- Education: Developed and co-taught a short course to identify technological, environmental, economic, political, and cultural issues related to energy decisions using both renewable and non-renewable technologies.

Graduate Research Assistant 2008 - 2010
Washington University in St. Louis, Laboratory for Advanced Combustion and Energy Research & Consortium for Clean Coal Utilization

Project: The effects of biomass cofiring on NOx emissions
- Utilized CFD to model flame structure and NOx emissions for coal and biomass cofired flames
- Identified flame structures that led to increased NOx emissions during air-fired and oxyfuel combustion
- Investigated coal devolatilization and post-combustion particle size using Thermogravimetric Analysis (TGA) and Electrical Low Pressure Impactor (ELPI)

Tsinghua University, Beijing, P.R. China

Project: Considerations for decision-making on distributed generation in rural areas (project in addition to dissertation research)

- Explored the feasibility of both renewable and fossil-fuel distributed power generation using both economic and social drivers for decision-making in developing countries without access to reliable electricity.
- Travelled to western rural China to see first-hand what rural herders use for electricity and what the implications of a distributed power generation facility would be.

Ph.D. First Year Program Rotations:
Washington University in St. Louis

Aerosol and Air Quality Research Laboratory Spring 2008

Research Advisor: Dr. Pratim Biswas
Project: Mercury removal using iodine based sorbents from coal-fired power plant exhaust gases

- Assessed the effectiveness of potassium iodide as a sorbent for mercury removal.
- Developed injection techniques for optimal mercury capture at different temperatures.
- Analyzed capture efficiency using an in situ elemental mercury analyzer, scanning mobility particle sizer (SMPS), and inductively coupled plasma mass spectrometry (ICP-MS).

Environmental Nanochemistry Laboratory Spring 2008

Research Advisor: Dr. Young-Shin Jun
Project: Observations of dissolution and precipitation of calcium carbonate using atomic force microscopy

- Studied the effects of fluid contact with natural surfaces abundant in potential CO₂ geological storage sites.
- Investigated dissolution rates of calcite and magnesite under ambient conditions at a neutral pH.
- Trained using in situ Atomic Force Microscopy imaging.


Washington University in St. Louis

Project: Sooting limits in diffusion flames

Developed a model to determine the effects of the stoichiometric mixture fraction on the sooting limits of oxygen-enriched laminar ethylene diffusion flames. Measured fuel velocity using Laser Doppler Velocimetry.

Formula Society of Automotive Engineers Design Competition Participant 2004 - 2007

Washington University in St. Louis

Project: Drivetrain/Braking Systems Lead

Worked an interdisciplinary team to design, fabricate, and test an integrated rear drivetrain (differential and A-arm mounting) and inboard braking system
Technical Skills

Software
* CFD: ANSYS Fluent, Gambit Mesh Generation, ANSYS Fluent Workbench
  * Advanced user with experience in gaseous and solid fuel combustion modeling; incompressible RANS and LES turbulence modeling; discrete phase models with lagrangian particle tracking; mesh generation; parallel processing; knowledge of turbulent-chemistry interaction models; and thorough knowledge of solid fuel combustion sub-models including devolatilization and char combustion
  * Completed Advanced user training at ANSYS FLUENT in Lebanon, NH (May 2009)

Other Computer Software and Programming Languages
* MATLAB, Solid Edge, C++, MathCAD, StressCheck (Finite Element Analysis)

Design
* Designed burner, combustion chamber, and particulate filter housing for a 35 kW coal/biomass furnace
* Designed flue gas recycle and blower system for oxy fuel combustion operation
* Constructed flow panel for flexible gas operation including air, oxygen, nitrogen, & carbon dioxide

Scientific Instruments
* Continuous emissions monitoring (CEM) analyzers for CO, CO₂, O₂, NOx, SOx, Hg, Thermogravimetric analyzer (TGA), scanning mobility particle analyzer (SMPS), inductively coupled plasma mass spectrometry (ICP-MS), atomic force microscopy (AFM), electrical low pressure impactor (ELPI)

Leadership Experience

- Member, Washington University Sustainability Advisory Committee 2011 - present
- Green Laboratory Initiative Representative Coordinator, Office of Sustainability 2011 – present
- Founder, Washington University Graduate Energy and Environment Network 2011 – present
- Planning Committee member, U.S. EPA STAR Conference of the Fellows 2011
- Student Representative, Washington University Board of Trustees 2010 - 2011
- Treasurer, Graduate and Professional Council (GPC) 2010 – 2011
- Member and Representative to GPC, Association of Graduate Engineering Students 2009 – 2010
- Member, Professional and Graduate Student Coordinating Committee (ProGradS) 2009 – 2010

Professional Experience

Laboratory Representative Coordinator: Green Labs Initiative 2011 - present
* Washington University Office of Sustainability
  * Led network of graduate students to reduce waste and electricity use in research laboratories.
  * Worked with cross-campus interdisciplinary taskforce to expand program to all labs and buildings.
  * Developed promotional materials and website to maintain communication and best practices.

Laboratory Safety Coordinator 2008 - present
* Washington University in St. Louis, Laboratory for Advanced Combustion and Energy Research
  * Complied with Washington University Environmental Health & Safety regulations and inspections.
  * Coordinated chemical storage and hazardous waste compliance.
  * Developed laboratory practices and standard operating procedures for seven flame and synthesis processes.
Vehicle Dynamics Development Engineer: 2009 Escape
Ford Motor Company, Dearborn, MI

- Applied comprehensive metrics to assess vehicle’s steering and road response performance.
- Improved ride, road noise, and steering by tuning lateral link bushings and sub-frame connections.
- Selected to attend driving school: Tier II certified driver.

Teaching & Mentorship Experience

Instructor
Energy Transfer Processes/Heat Transfer (ChE 369/MEMS 342)
Spring 2013

Guest Lecturer
Energy Transfer Processes/Heat Transfer (ChE 369/MEMS 342)
Spring 2012

Teaching Assistant
Heat Transfer/Energy Transfer Processes (ChE 369/MEMS 342)
Spring 2009
Combustion Phenomena (EECE 5404)
Fall 2009
Engineering Analysis of Chemical Systems (ChE 351)
Fall 2008

Senior Design & Independent Study Project Coordinator
Mechanical Engineering Senior Design Project & Independent Study (MEMS 411/MEMS 400)
Fall 2007

Student Member, Committee for EECE Faculty Recruitment
Spring 2009 & 2010

Publications

4. Holtmeyer, ML, Kumfer, BM, Axelbaum, RL. Predicting the volatile flame length for coal and biomass cofired flames. (In progress)
5. Li G, Holtmeyer ML, Axelbaum RL, Li S. Flame length impacts on fly ash characteristics and deposition during air-fired and oxyfuel combustion of coal and biomass. (In progress)

Conference Presentations


• Skeen SA, Holtmeyer ML, Kumfer BM, Axelbaum RL. Effects of particle size and nitrogen content on nitrogen oxide formation during biomass co-firing. The Central States Section of the Combustion Institute 2010. Urbana-Champaign, Illinois


• Holtmeyer ML, Skeen SA, Kumfer BM, Axelbaum RL. Nitric oxide emissions during coal and coal/biomass combustion under air-fired and oxy-fuel conditions. 2010 American Institute of Chemical Engineers Annual Meeting 2010. Salt Lake City, Utah

• Holtmeyer ML, Axelbaum RL. “Fundamental flame studies applied to oxyfuel combustion of biomass and coal to reduce pollutant formation”. Missouri Space Grant Consortium Annual Meeting. April 2011. St. Louis, Missouri


• Holtmeyer ML, Kumfer BM, Axelbaum RL. “The effects of biomass cofiring on flame structure and NO formation during air-fired and oxy-fuel combustion”. 2nd Oxyfuel Combustion Conference. 12-16 September 2011. Queensland, Australia


• Holtmeyer ML, Kumfer BM, Axelbaum RL. “The effects of biomass cofiring on flame structure and NO formation in air-fired and oxy-fuel combustion”. AICHE Annual Meeting. 16-21 October 2011. Minneapolis, Minnesota


• (Poster Presentation) Holtmeyer ML, Li G, Kumfer BM, Li S, Axelbaum RL. Characteristics of biomass fuels and their impact on volatile flame length during biomass cofiring combustion. 34th International Symposium on Combustion. Warsaw, Poland


Awards, Honors and Academic Affiliations

Speaking Engagements

• Selected to deliver student speech at Brauer Hall Dedication, 2010
• Selected to deliver student speech at Brauer Hall Groundbreaking Ceremony, 2008
• Washington University Engineering Alumni Connection Series Invited Speaker, 2008
• Student Presenter at the MAGEEP Doctoral Network, Hong Kong, 2008
Awards

• First runner-up for Best Student Paper Award at 36th International Technical Conference on Coal and Fuel Systems, Clearwater, FL, 2011
• Graduate & Professional Council's Bridging GAPS award for Sustainability, 2011
• Outstanding Student Presenter at Central States Combustion Institute Meeting, Tuscaloosa, AL, 2008
• Endowed Charles and Marlene Buescher Scholarship for Energy and Environment, 2007
• Pi Beta Phi Sorority (Thurtene Carnival Construction Overall and Burmeister Cup Winner), 2007
• Outstanding Mechanical Engineering Senior Design Project, 2005
• Dean’s Scholar, 2002-2006

Academic Affiliations

• American Institute of Chemical Engineers, 2010 - present
• Tau Beta Pi (Engineering Honorary), inducted Spring 2006
• Pi Tau Sigma (Mechanical Engineering Honorary), inducted Spring 2006
• Society of Women Engineers (Publicity Chair), 2004
• Society of Automotive Engineers (SAE), 2004 - 2007

References

Richard L. Axelbaum, Ph.D
Research Advisor, Stifel & Quinette Jens Professor of Environmental Engineering Science, Department of Energy, Environmental, & Chemical Engineering
Campus Box 1180
One Brookings Drive
St. Louis, MO 63130
314.935.7560
axelbaum@wustl.edu

Pratim Biswas, Ph.D.
Chair, Department of Energy, Environmental & Chemical Engineering
Lucy & Stanley Lopata Professor
Campus Box 1180
One Brookings Drive
St. Louis, MO 63130
314.935.5548
Pratim.biswas@wustl.edu

Elaine Berland, Ph.D.
Associate Dean of the Graduate School of Arts & Sciences, Director of the Graduate Center Director of Graduate Affairs
Campus Box 1186
One Brookings Drive
St. Louis, MO 63130
314.935.7355
berland@wustl.edu